

Supporting Information for:

Accelerating Discovery Through Integration: A DFT validated Machine Learning Framework for Screening MOF Photocatalysts

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S1: Detailed Computational Methods

1.1 DFT Calculation Parameters

All Density Functional Theory (DFT) calculations were performed using the Vienna Ab initio Simulation Package (VASP, version 6.4.3). The electronic structure was determined using the HSE06 (Heyd-Scuseria-Ernzerhof) hybrid functional, incorporating 25% exact Hartree-Fock exchange with a range-separation screening parameter of $0.2 \text{ \AA}^{-1}$, and used a energy cut-off of 520 eV. We used the standard Projector-Augmented-Wave (PAW) potentials provided with the VASP package. The k-point mesh for sampling the Brillouin zone was generated using the vaspkit package to ensure consistent sampling density across the diverse unit cells. We used the Gamma centered Monkhorst-Pack scheme with a reciprocal cell of $2\pi \times 0.04 \text{ \AA}^{-1}$.

Note on Methodology: Single-Point HSE06 on PBE relaxed geometries The electronic properties reported in this work were obtained via single-point HSE06 calculations performed on geometries previously relaxed using the PBE (Perdew-Burke-Ernzerhof) functional. Full structural relaxation using hybrid functionals is computationally very expensive and limiting for high-throughput screening of thousands of MOFs. However, PBE is widely recognized for predicting MOF structural parameters with reasonable accuracy, despite its primary limitation being the underestimation of bandgaps. By applying the HSE06 functional to PBE-optimized geometries, we correct the electronic structure description (specifically bandgaps and band edge positions) to a level comparable to full hybrid optimization, but at a fraction of the computational cost. The error introduced by neglecting hybrid-level structural relaxation is expected to be negligible compared to the significant improvement in electronic property prediction.

1.1.1 VASP INCAR Tags (HSE06)

Key parameters used for the HSE06 hybrid functional single-point calculations in VASP.

Global Parameters

SYMPREC = 1.00e-08 (Symmetry precision)
LCHARG = .TRUE. (Write CHGCAR or not)
LAECHG = .TRUE. (Writes the reconstructed all-electron charge density)
ADDGRID = .TRUE. (Increase grid, helps GGA convergence)
LASPH = .TRUE. (Give more accurate total energies and band structure calculations)
LVHAR = .TRUE. (Write ionic + Hartree electrostatic potential into LOCPOT or not)
LWAVE = .TRUE. (Write WAVECAR or not)

Computational Parameters

KPAR = 1 (Divides k-grid into separate groups)
NSIM = 16 (Number of bands optimized simultaneously)
NCORE = 1 (Number of cores per orbital)

Static Calculation

ISMEAR = 0 (Gaussian smearing method)
SIGMA = 0.010000 (Width of the smearing, in eV)
LORBIT = 11 (PAW radii for projected DOS)
NEDOS = 2001 (DOSCAR points)
NELM = 150 (Max electronic SCF steps)
EDIFF = 1.00e-05 (SCF energy convergence, in eV)
ENCUT = 520.000 (Energy cutoff for the plane-wave basis set, in eV)
GGA = PE (Specifies the GGA functional to use)
ISYM = 3 (Symmetry flag)

DFT-D3

IVDW = 12 (Selects the van der Waals correction method)
VDW_S8 = 2.310000 (Damping parameter s8 in the D3 correction)
VDW_A1 = 0.383000 (Damping parameter a1 in the D3 correction)
VDW_A2 = 5.685000 (Damping parameter a2 in the D3 correction)

HSE06

LHFCALC = .TRUE. (Enables hybrid functional calculations)
AEXX = 0.25 (Fraction of exact Hartree-Fock exchange, 25% for HSE06)
HFSCREEN = 0.2 (Screening parameter for the short-range exchange in HSE functionals)
ALGO = All (Electronic minimization algorithm)
PREC = Accurate (Precision level for calculations)

1.2 Machine Learning Model Details

1.2.1 Molecular Graph Transformer (MGT) Hyperparameters

The following hyperparameters were used for training the MGT model.

- **Graph Construction & Featurization**
 - **Atomic Descriptor Vector Length:** 90
 - **Local Cutoff Radius:** 8 Å
 - **Global Cutoff Radius:** 12 Å
 - **Maximum Neighbors per Atom (Local Graph):** 12
 - **Radial Basis Function (RBF) Bins:**
 - 80 for bond lengths
 - 40 for bond angles
 - 120 for Coulomb interactions
- **Network Architecture**
 - **MGT Encoder Layers:** 1 layer
 - **Convolutional Layers per Encoder:**
 - 3 Angle
 - 3 Bond
 - 1 Electrostatic
 - **Embedding Layer Dimensionality:** 128
 - **Hidden Layer Dimensionality:** 512
- **Training & Optimization**
 - **Optimizer:** Adam
 - **Loss Function:** Mean Squared Error (MSE)
 - **Learning Rate:** 1×10^{-4}
 - **Weight Decay:** 1×10^{-5}
 - **Training Duration:** 200 epochs
 - **Effective Batch Size:** 16 (Base batch size of 2 with 8 gradient accumulation steps)

1.2.2 Training and Validation Loss

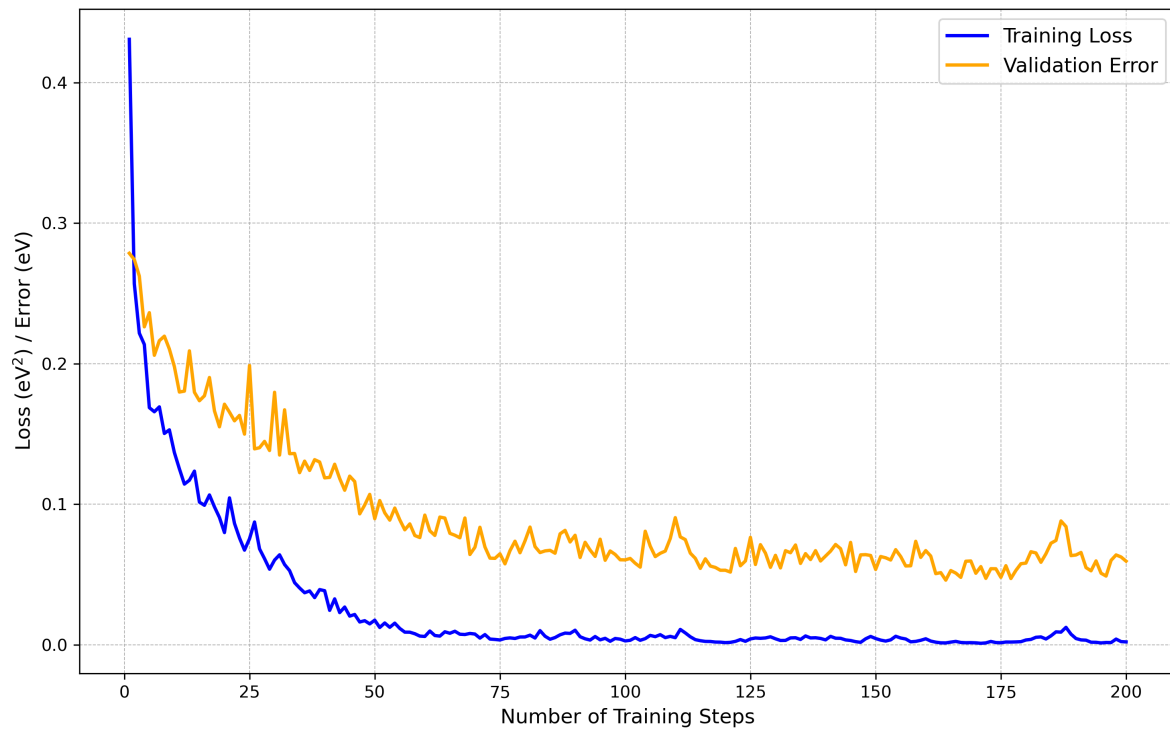


Figure S1: Training and validation loss curves for the MGT model over the training epochs. This plot demonstrates model convergence and the absence of significant overfitting.

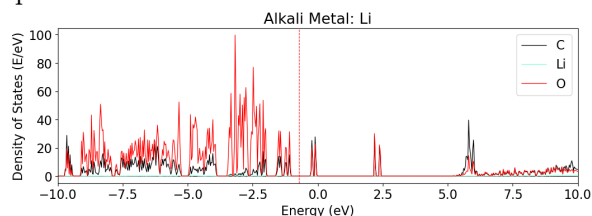
S2: Additional Electronic Structure Analysis

2.1 Projected Density of States (pDOS) for DFT Candidates

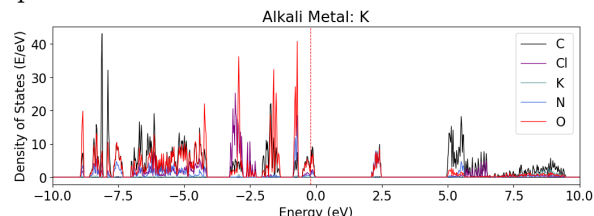
2.1.1 Alkali

Figure S2: pDOS plots for all structure containing an Alkali metal

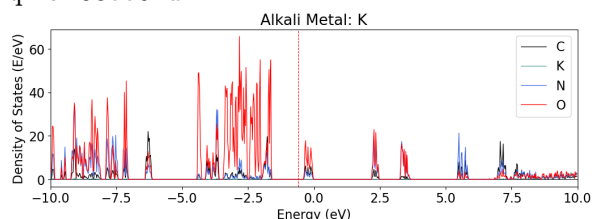
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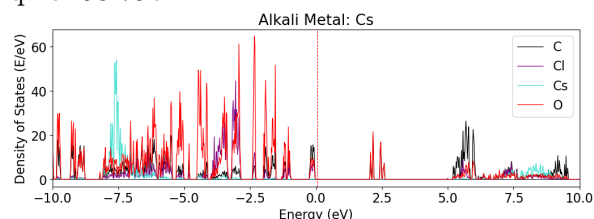
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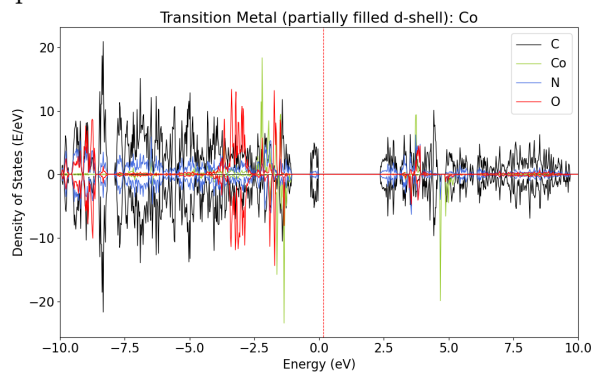
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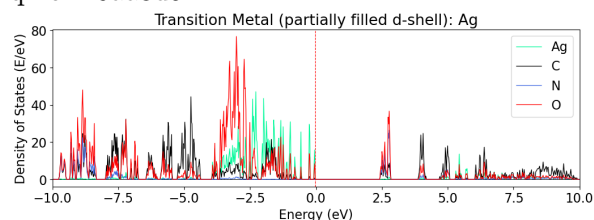
2.1.2 Transition Metals with Partially Filled d-Shells

Figure S3: pDOS plots for all structure containing a Transition metal with most common ions whose d-shell is only partially filled

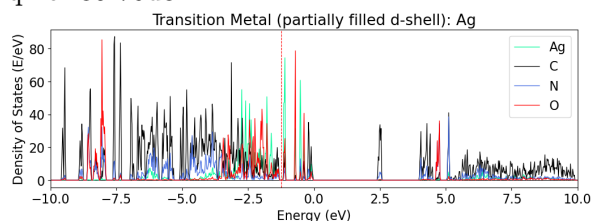
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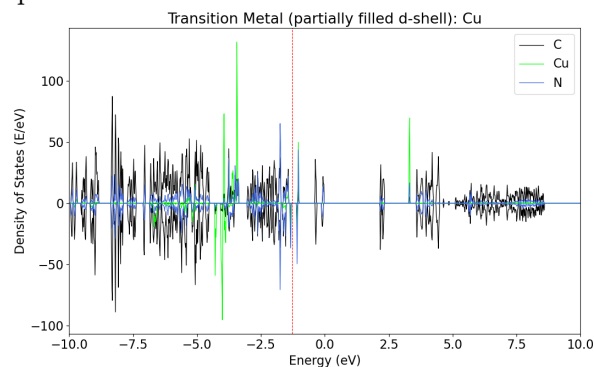
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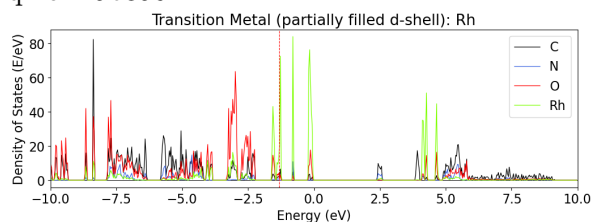
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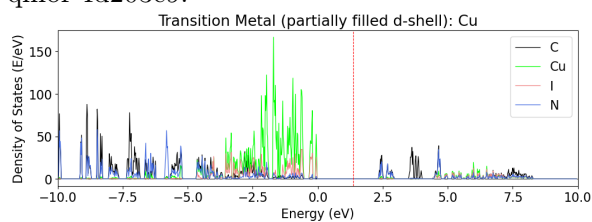
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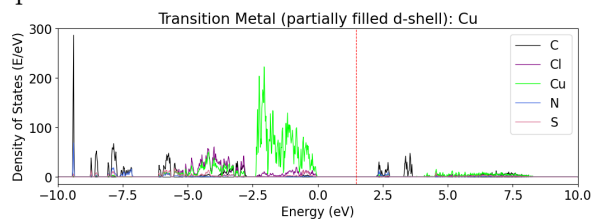
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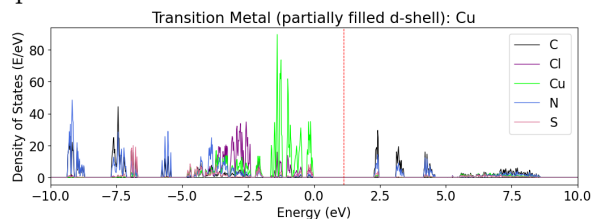
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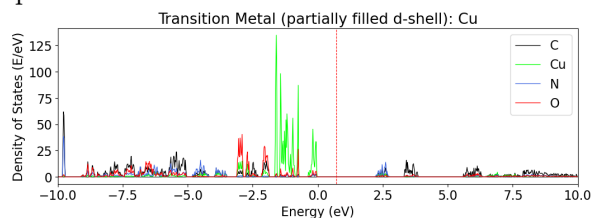
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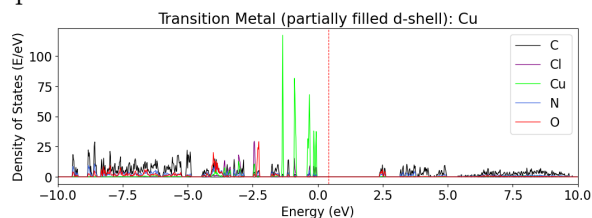
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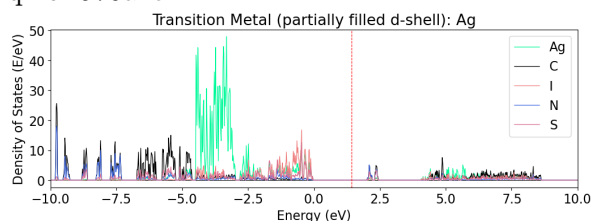
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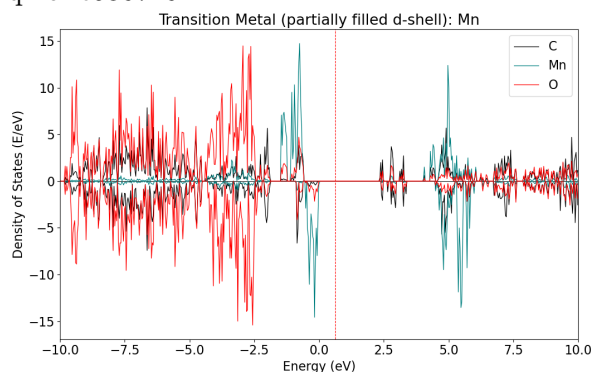
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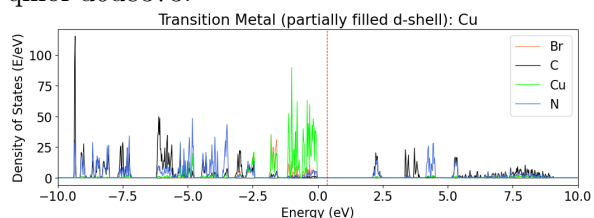
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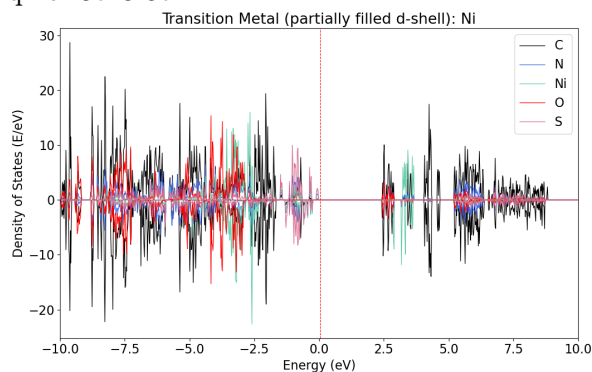
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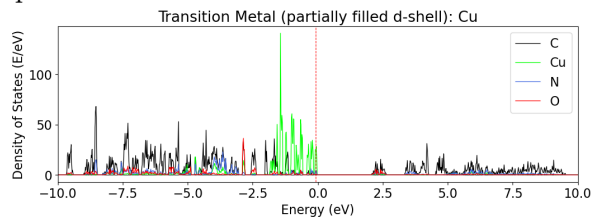
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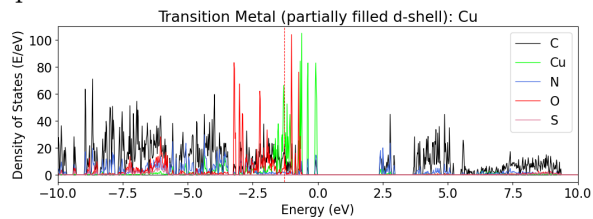
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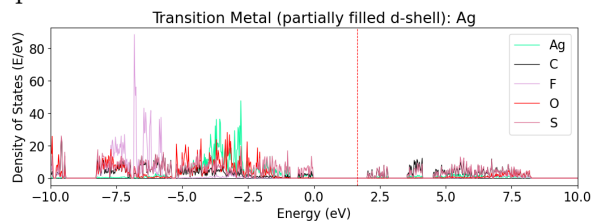
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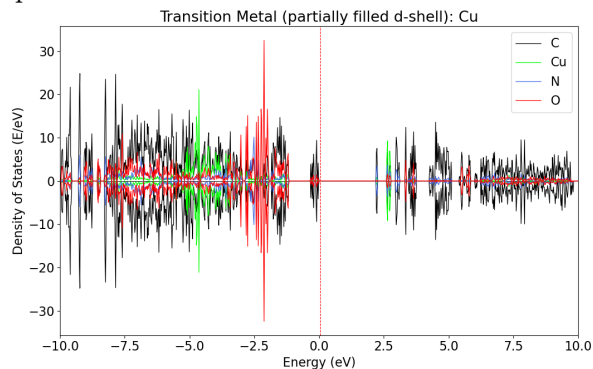
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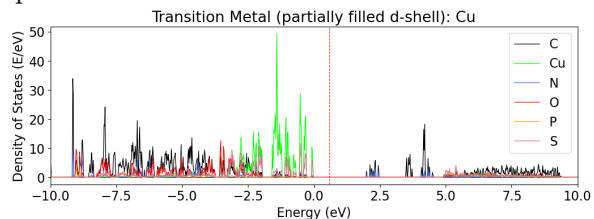
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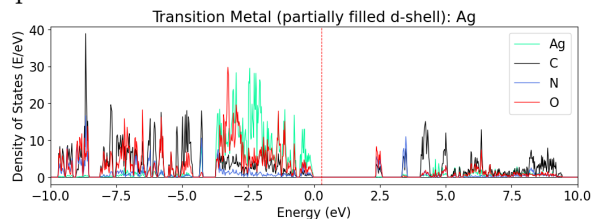
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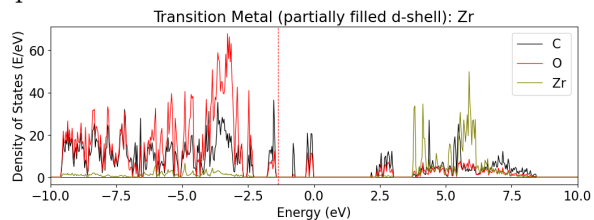
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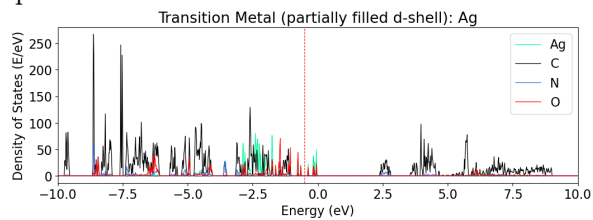
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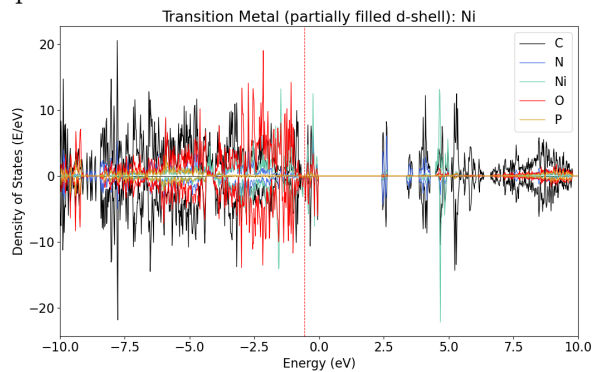
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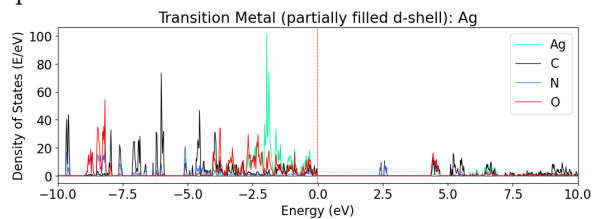
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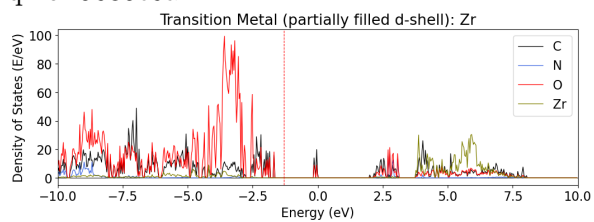
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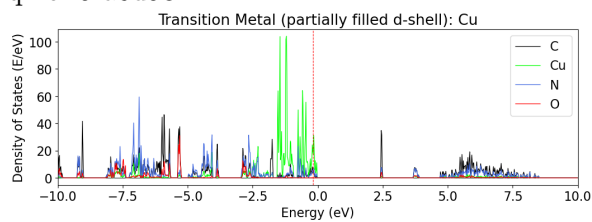
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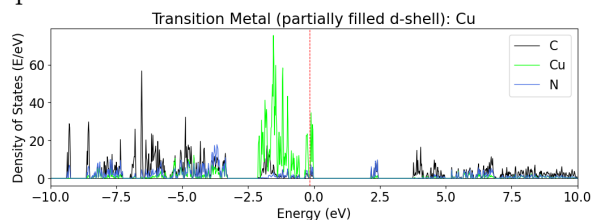
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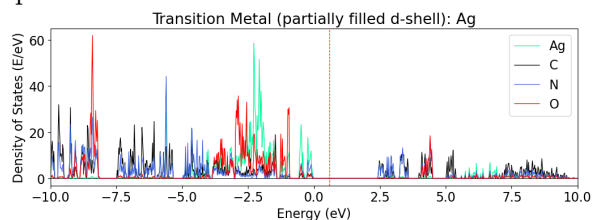
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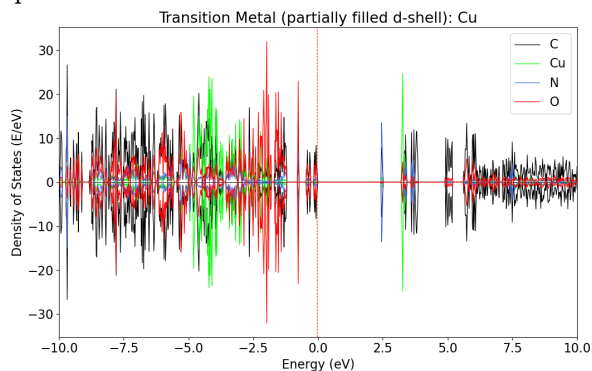
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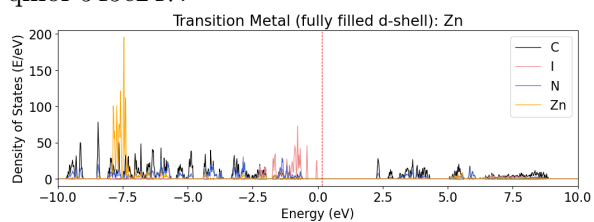
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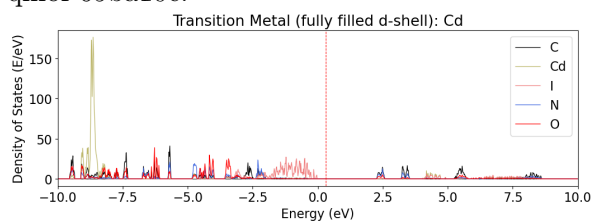
2.1.3 Transition Metals with Fully Filled d-Shells

Figure S4: pDOS plots for all structure containing a Transition metal with most common ions whose d-shell is fully filled

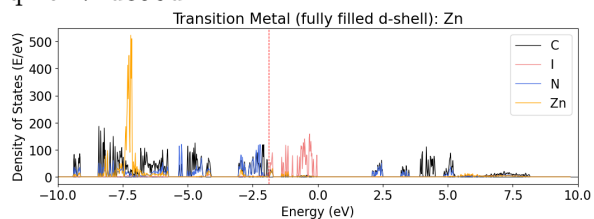
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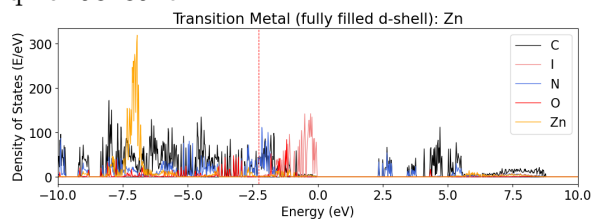
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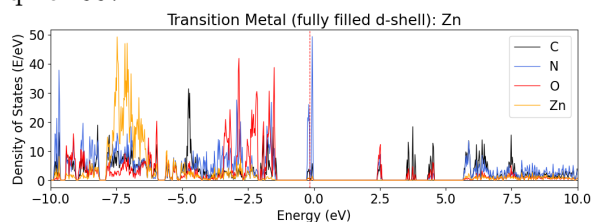
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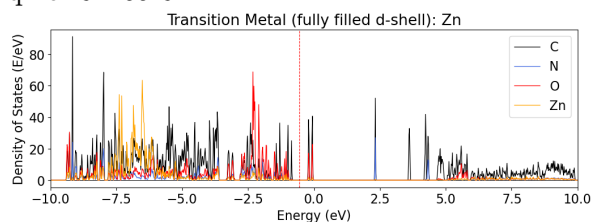
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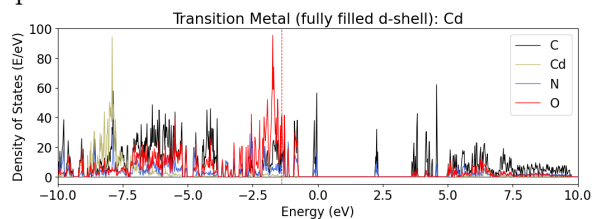
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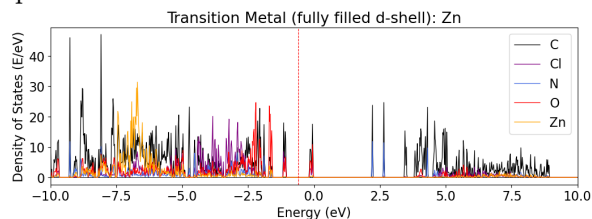
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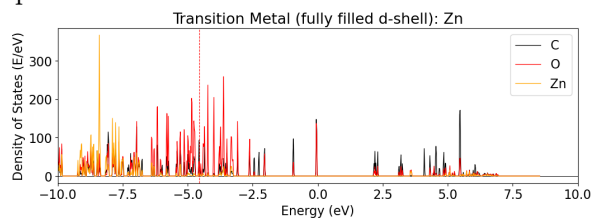
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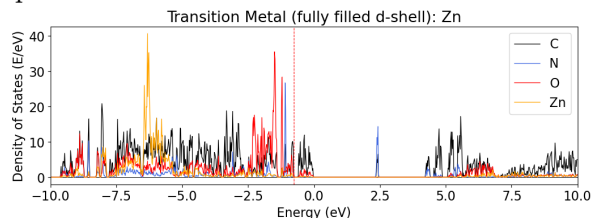
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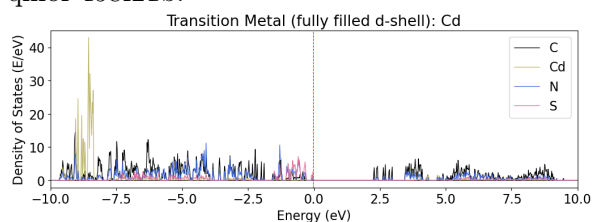
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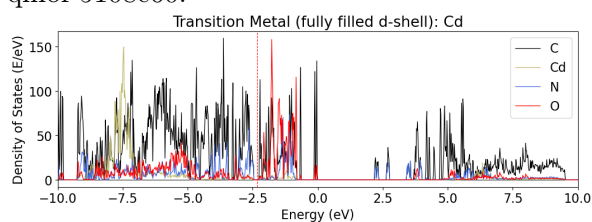
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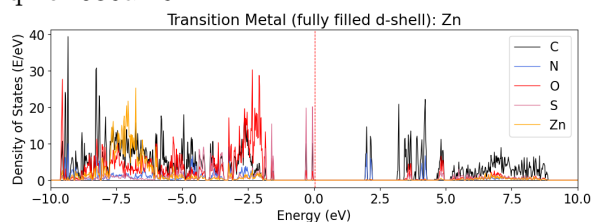
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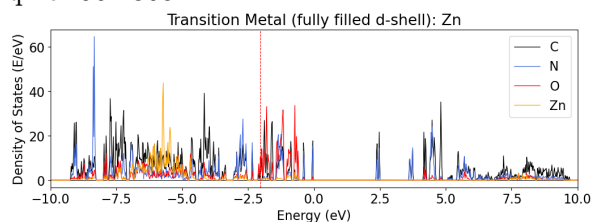
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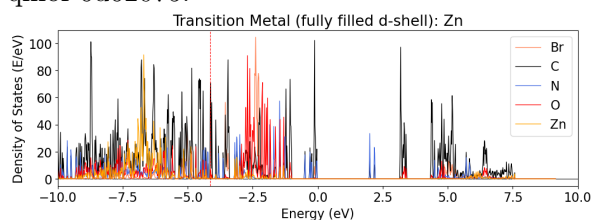
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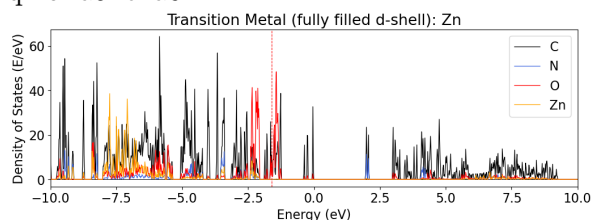
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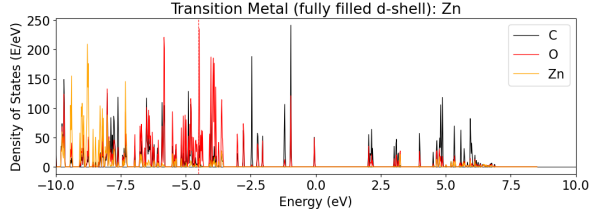
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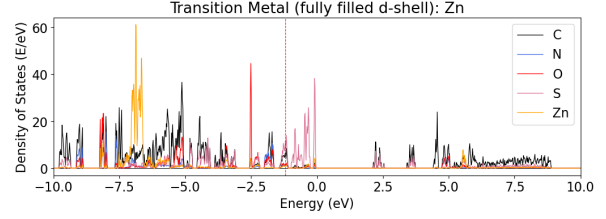
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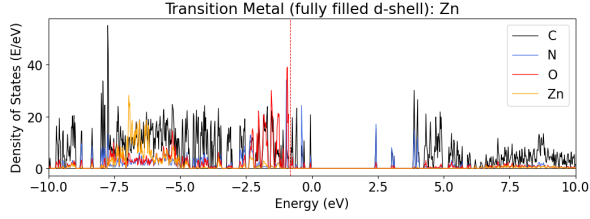
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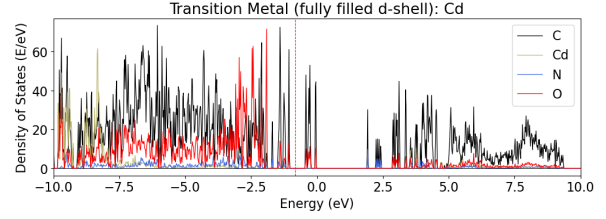
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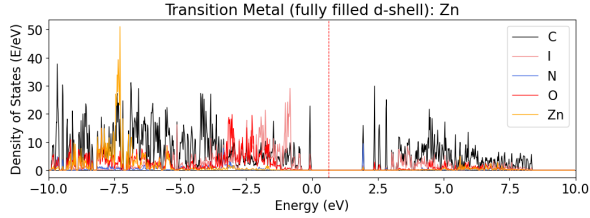
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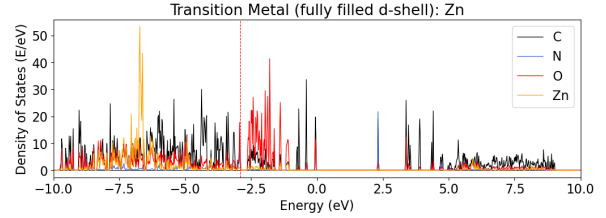
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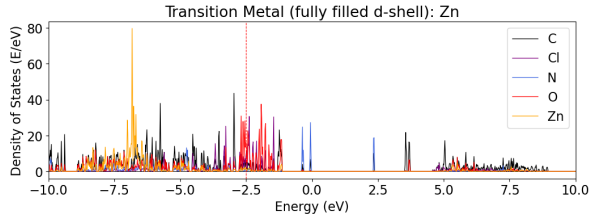
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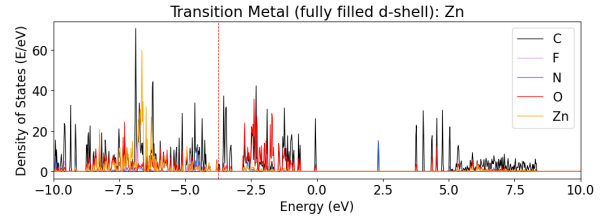
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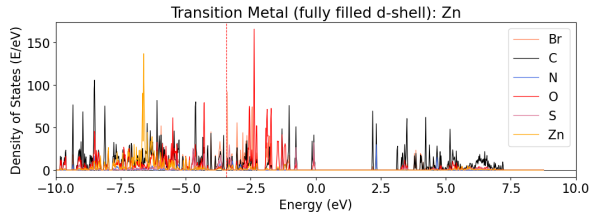
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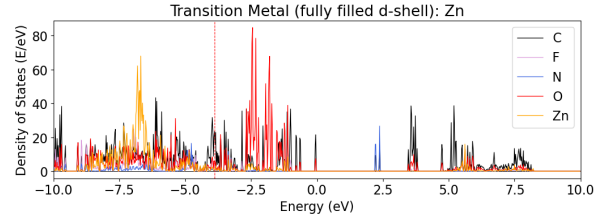
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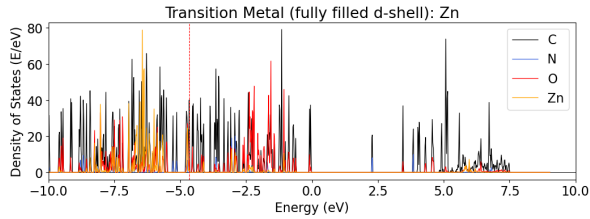
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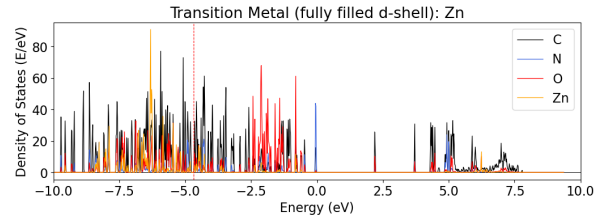
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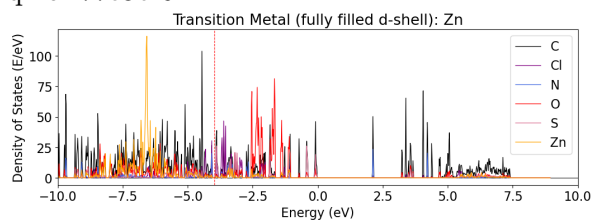
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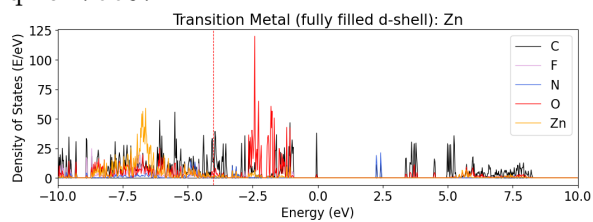
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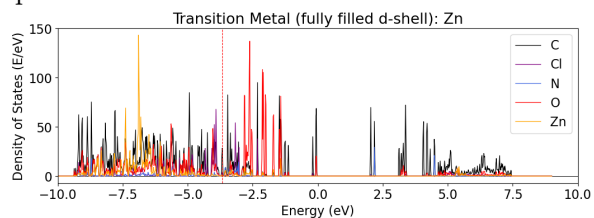
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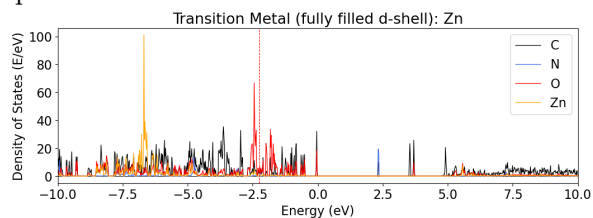
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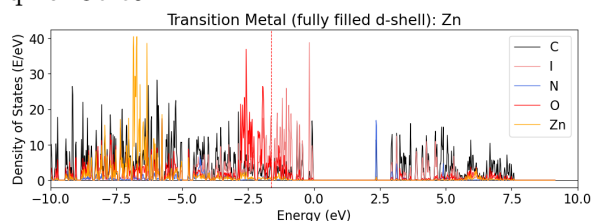
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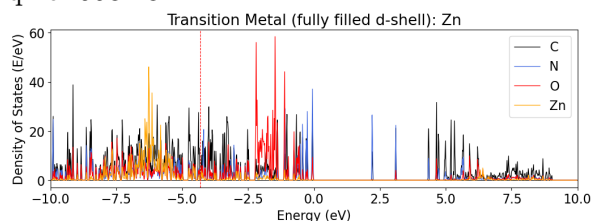
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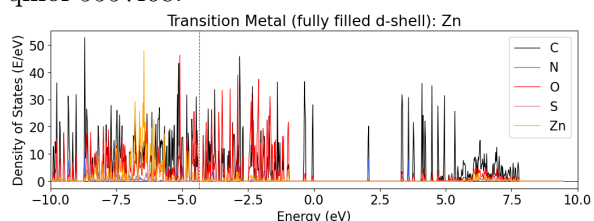
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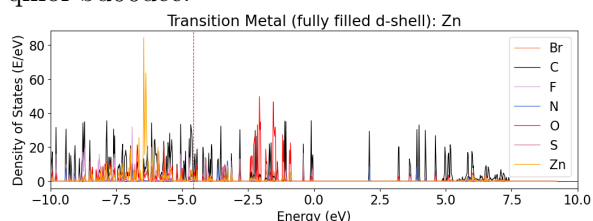
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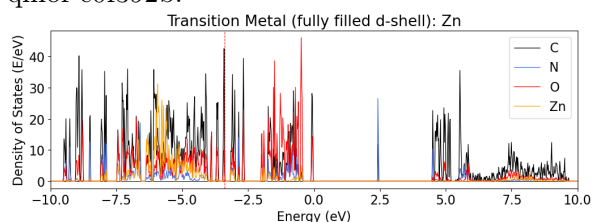
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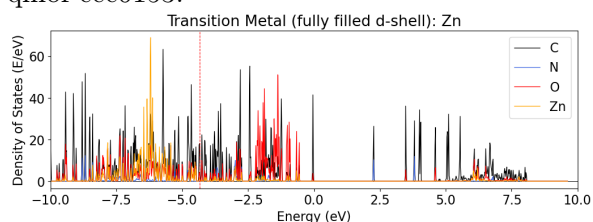
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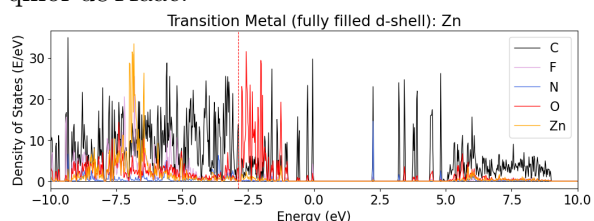
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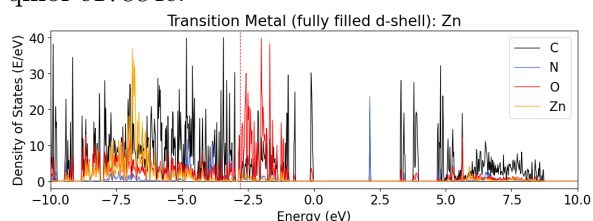
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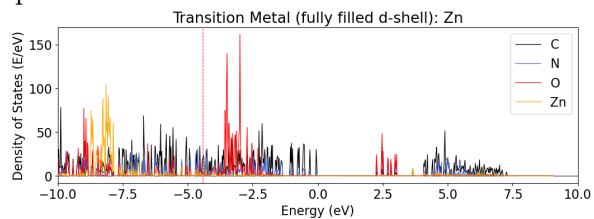
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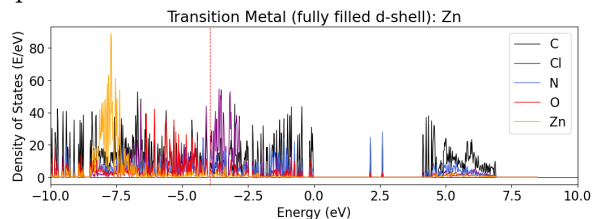
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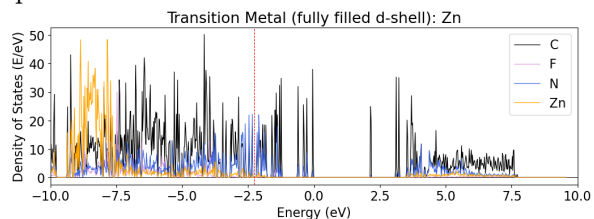
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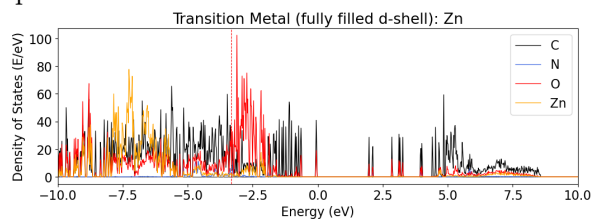
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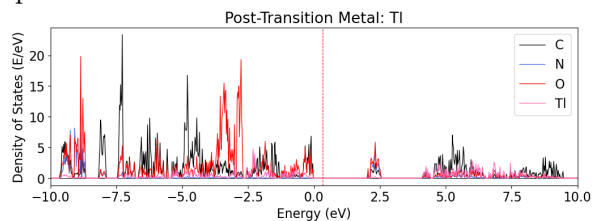
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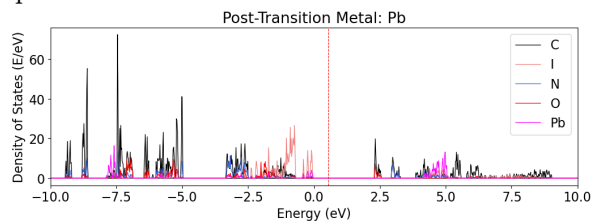
2.1.4 Post-Transition Metals

Figure S5: pDOS plots for all structure containing a Post-Transition metal

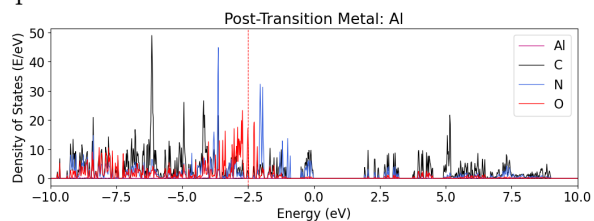
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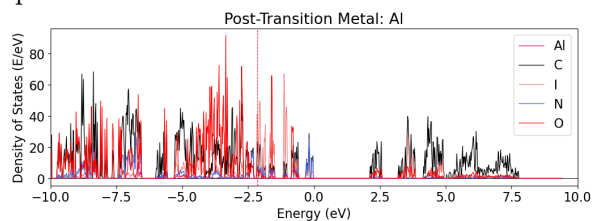
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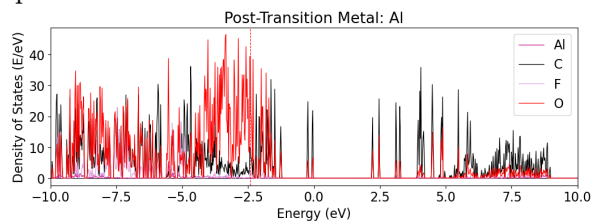
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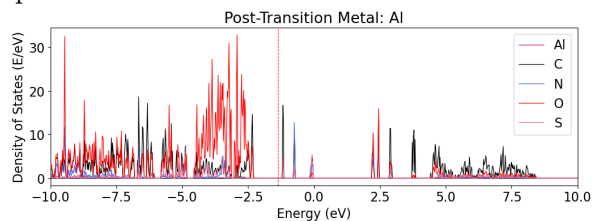
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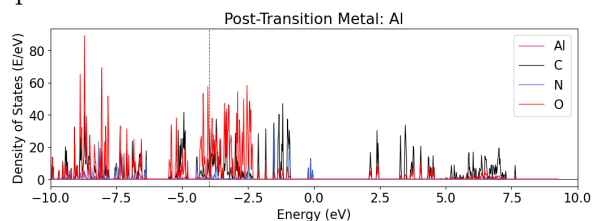
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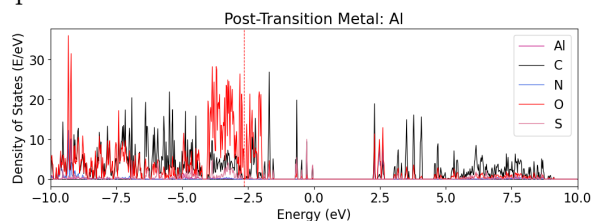
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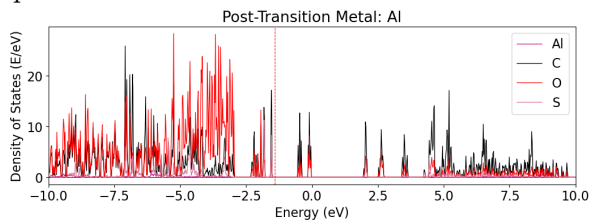
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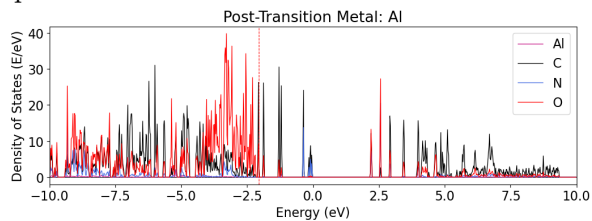
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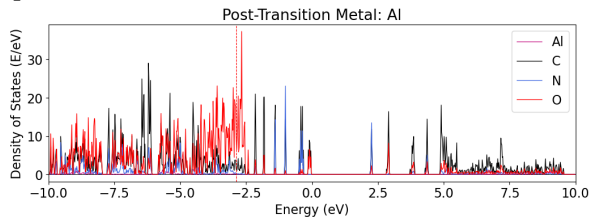
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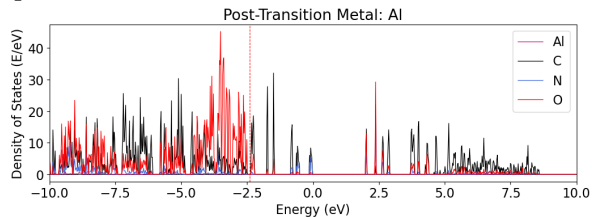
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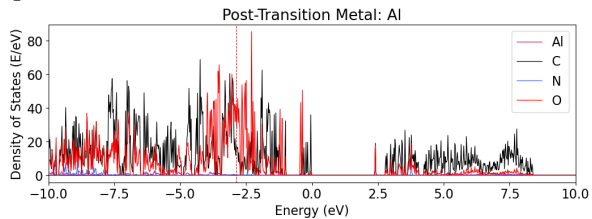
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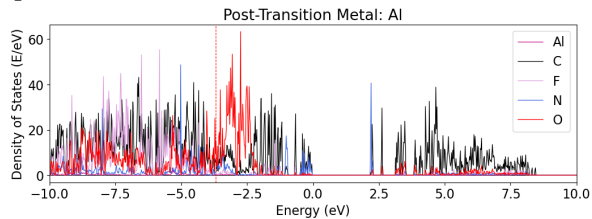
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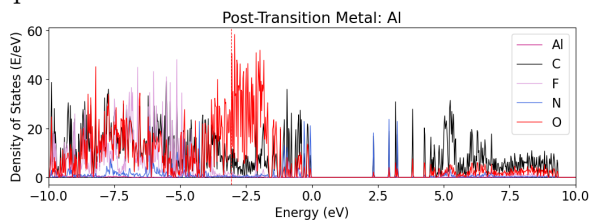
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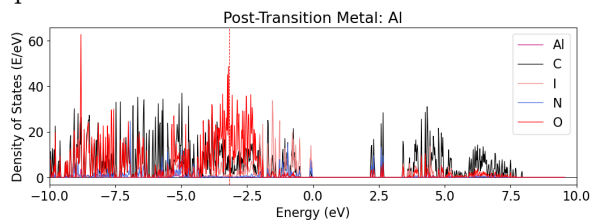
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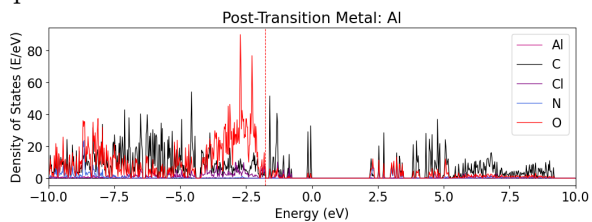
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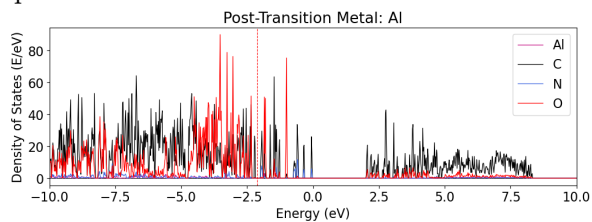
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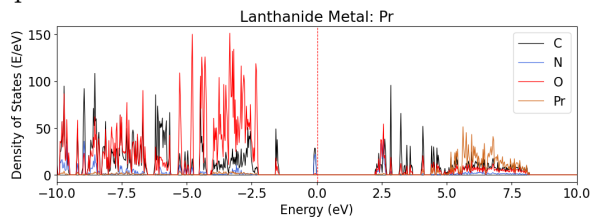
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2.1.5 Lanthanides

Figure S6: pDOS plots for all structure containing a Lanthanide metal

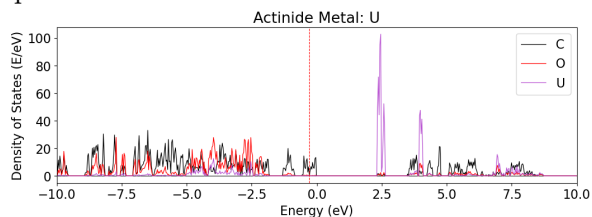
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2.1.6 Actinides

Figure S7: pDOS plots for all structure containing an Actinide metal

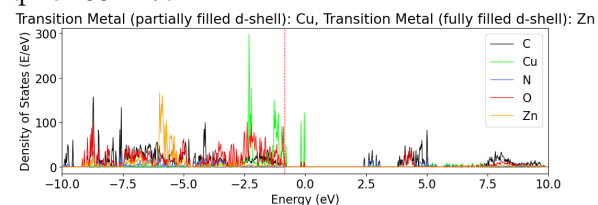
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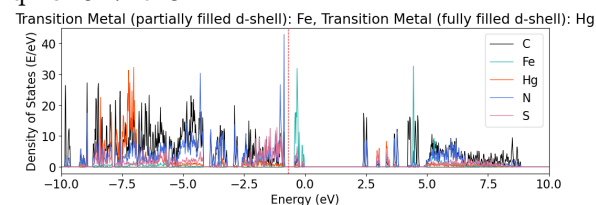
2.1.7 Multi-Metal

Figure S8: pDOS plots for all structure containing multiple metals in their metal centres

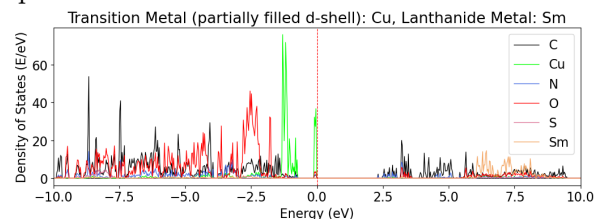
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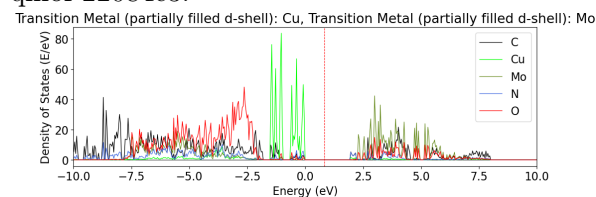
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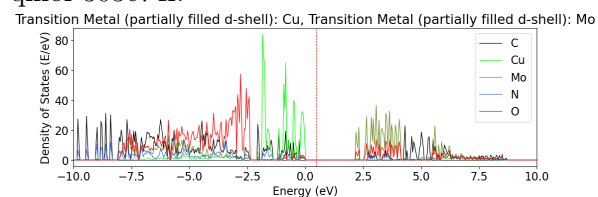
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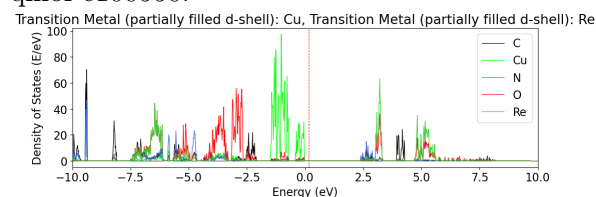
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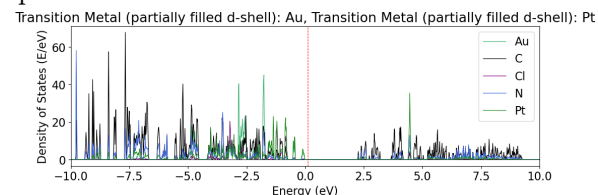
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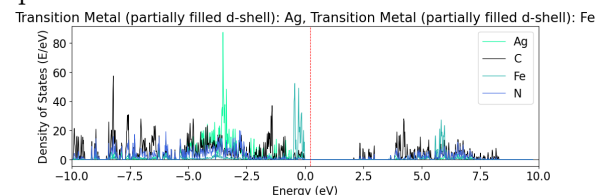
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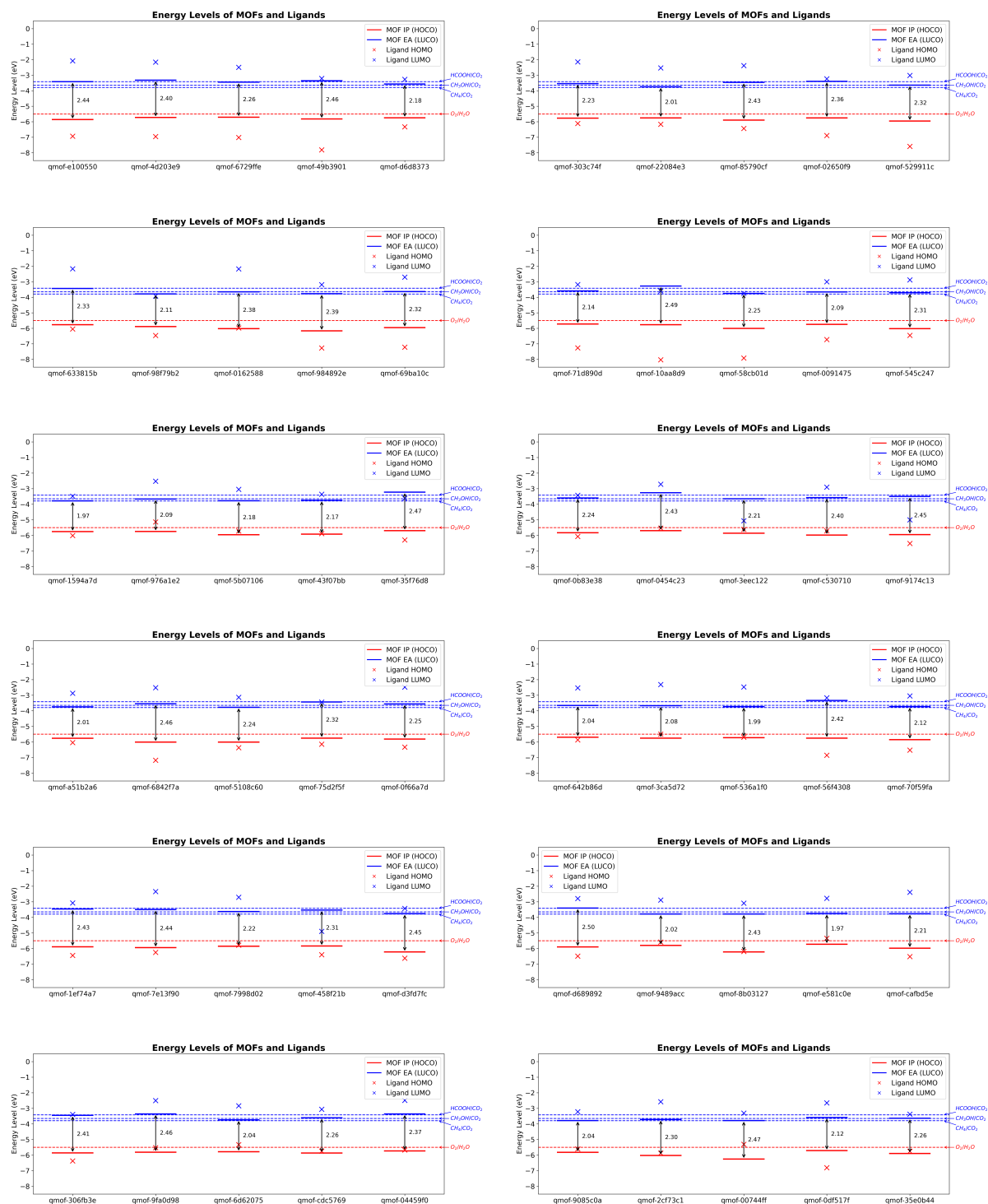


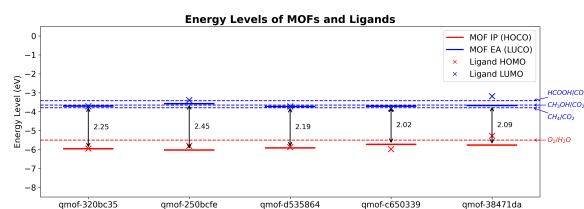
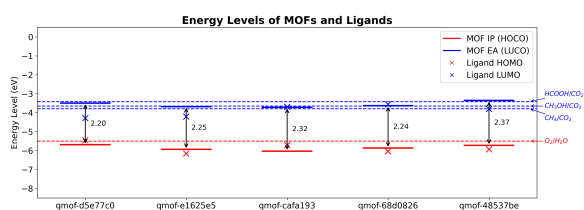
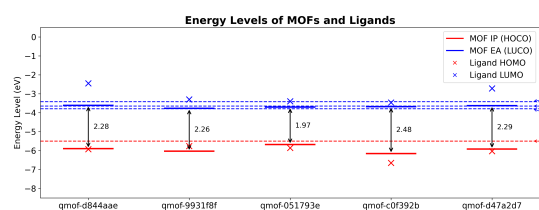
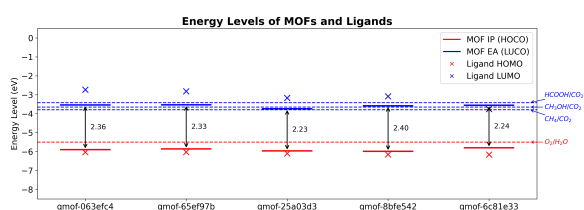
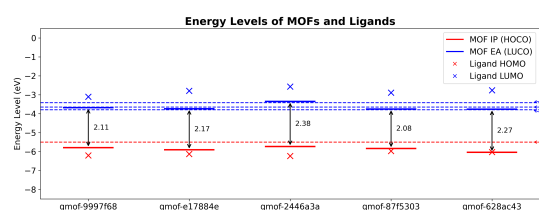
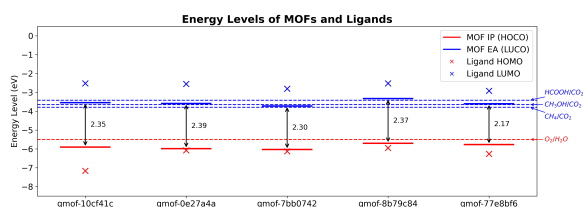
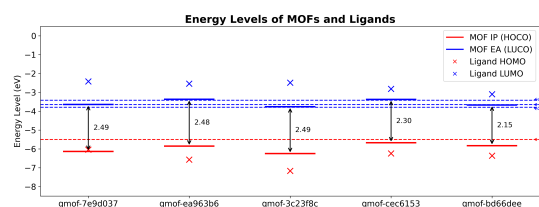
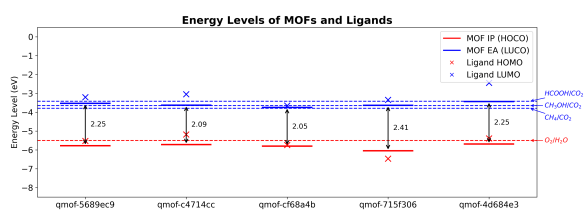
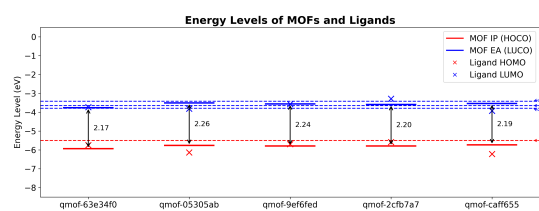
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2.2 Energy Diagrams for DFT Candidates

Figure S9: Energy diagrams comparing the Highest Occupied Crystal Orbital (HOCO) and Lowest Unoccupied Crystal Orbital (LUCO) of each MOF with the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) defined by the ligands of the MOF. For MOFs with multiple ligand types the HOMO and LUMO are taken as the highest HOMO and lowest LUMO between all of the ligands





S3: Extended Machine Learning Performance Analysis

A detailed assessment of the model’s performance on the test set is provided in Table S1, where the Mean Absolute Error (MAE), Root Mean Squared Error (RMSE) and the Coefficient of Determination (r^2) are used to show the predictive ability of the model.

$$MAE = \frac{1}{n} \sum_{i=1}^n |x_i - y_i| \quad (1)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n |x_i - y_i|^2}{n}} \quad (2)$$

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} = 1 - \frac{\sum_{i=1}^n |x_i - y_i|^2}{\sum_{i=1}^n |x_i - \bar{x}|^2} \quad (3)$$

Where x_i and y_i are the DFT-calculated and MGT-predicted values of MOF_i respectively, $\bar{x}$ is the mean of the truth values and n is the number of MOFs in the test set.

The MAE is the most direct measure of the average prediction error, representing the average difference between the MGT-predicted and DFT-calculated values. The RMSE, similar to the MAE, is a measure of the average prediction error, however, due to its squaring of the error terms it is particularly sensitive to outlier predictions with large errors. The R^2 , on the other hand, provides a normalised value that described how well the variance in the DFT-calculated values is explained by the MGT model, therefore serving as a measure of the model’s predictive power, with values closer to 1 indicating a more robust model.

Table S1: Detailed error metrics for the three predicted electronic properties on the test set, which demonstrate the model’s robust predictive capability. For all three properties, the RMSE is substantially lower than the corresponding standard deviation, confirming the model’s utility. The model performs best for the bandgap prediction, where it achieves the highest R^2 of 0.67. This value indicates that the model explains a significant portion of the property’s variance, implying that it has learned some of the underlying physics that determine the bandgap.

Property	Mean (eV)	Standard Deviation (eV)	MAE (eV)	RMSE (eV)	R^2
Bandgap	2.872245764	0.758242084	0.303129297	0.432928606	0.674000603
IP	6.079553202	0.776472963	0.37818499	0.528469579	0.536779994
EA	3.207307444	0.705470045	0.361087653	0.488914593	0.519704137

Table S2: Average errors for ML predictions categorized by metal. The results show that the model’s accuracy is linked to the metal’s electronic complexity. Higher prediction errors are consistently observed for d-block elements like Cobalt (Co), Palladium (Pd), and Technetium (Tc), and f-block elements such as Cerium (Ce), Ytterbium (Yb), and Actinium (Ac)

Metal		Bandgap (eV)	IP (eV)	EA (eV)	Overall (eV)
Alkali	K	0.244	0.408	0.416	0.356
	Cs	0.174	0.141	0.278	0.197
	Na	0.686	0.536	0.794	0.672
	Li	0.383	0.466	0.477	0.442
	Rb	0.296	0.050	0.308	0.218
Alkaline	Ba	0.188	0.096	0.175	0.153
	Mg	0.292	0.288	0.075	0.219
	Ca	0.616	0.713	0.208	0.512
	Sr	0.394	0.255	0.170	0.273
Transition (Partial)	Cu	0.305	0.361	0.353	0.340
	Ni	0.438	0.399	0.398	0.412
	Co	0.441	0.399	0.488	0.443
	Mn	0.310	0.246	0.370	0.309
	Fe	0.269	0.479	0.376	0.375
	Mo	0.203	0.212	0.258	0.224
	Ag	0.216	0.425	0.438	0.360
	V	0.187	0.374	0.265	0.275
	Pt	0.248	0.349	0.446	0.348
	Y	0.845	0.503	0.449	0.599
	Pd	0.682	0.284	0.620	0.528
	Tc	0.523	0.575	1.075	0.724
	Au	0.253	0.568	0.660	0.494
	W	0.185	0.526	0.554	0.422
	Zr	0.189	0.758	0.728	0.558
	Rh	0.285	0.358	0.386	0.343
	Hf	0.321	0.131	0.151	0.201
	Cr	1.142	0.137	1.035	0.771
	Ti	0.419	0.520	0.138	0.359
	Re	0.072	0.498	0.566	0.379

Table S2 – continued from previous page

Metal		Bandgap (eV)	IP (eV)	EA (eV)	Overall (eV)
Transition (Filled)	Zn	0.239	0.255	0.317	0.270
	Cd	0.301	0.591	0.624	0.505
	Hg	0.344	0.517	0.696	0.519
Post-Transition	Al	0.224	0.286	0.345	0.285
	Pb	0.147	0.237	0.366	0.250
	Ga	1.100	0.549	0.574	0.741
	Tl	0.059	0.618	0.703	0.460
	Bi	0.167	0.232	0.445	0.281
Metalloids	B	0.320	0.336	0.357	0.338
	Si	0.531	0.315	0.355	0.400
Lanthanides	Tb	0.173	0.232	0.029	0.145
	La	0.352	0.150	0.144	0.215
	Gd	0.220	0.163	0.294	0.226
	Nd	0.121	0.210	0.135	0.155
	Dy	0.028	0.035	0.052	0.039
	Ho	0.049	0.078	0.016	0.048
	Sm	0.219	0.128	0.208	0.185
	Pr	0.422	0.388	0.370	0.393
	Er	0.183	0.301	0.225	0.236
	Ce	0.367	1.172	0.960	0.833
	Yb	3.236	1.779	1.566	2.194
Actinides	U	0.301	0.364	0.354	0.339
	No	0.311	0.379	0.116	0.269
	Ac	1.100	0.549	0.574	0.741

S4: Complete Screening Results and Candidate Lists

Table S3: Complete list of the HSE06 calculation results for the 2,169 MOF structures selected from the initial screening, and suitability for each CO₂ reduction reaction considered in this paper.

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-019ba28	-3.066844462	-5.370394462	2.30355			
qmof-61fda9f	-2.143495384	-4.910977384	2.767482			
qmof-34d7993	-2.350993484	-5.701931484	3.350938			
qmof-d529df5	-2.911311632	-6.841083632	3.929772			
qmof-868b2eb	-2.475134487	-5.046014487	2.57088			
qmof-9ceb223	-2.889852972	-7.087535972	4.197683			
qmof-1d25033	-2.452318233	-6.004157233	3.551839			
qmof-51b139b	-2.665159685	-6.059279685	3.39412			
qmof-fb7f2ef	-2.151791163	-5.283315163	3.131524			
qmof-d55908c	-2.608338717	-5.109537717	2.501199			
qmof-5d009d5	-2.278155805	-6.862183805	4.584028			
qmof-c939f55	-2.940822672	-5.545498672	2.604676			
qmof-8f721fc	-2.804855335	-6.130434335	3.325579			
qmof-0b3d138	-2.232426148	-6.085495148	3.853069			
qmof-5718ab1	-2.401216969	-6.220476969	3.81926			
qmof-f0bdd71	-1.945316817	-5.715274817	3.769958			
qmof-7a182f0	-2.414688793	-5.690908793	3.27622			
qmof-afc3059	-3.493727762	-6.365559762	2.871832			
qmof-61282f6	-2.725546642	-6.392615642	3.667069			
qmof-225c8dd	-4.149858547	-6.287654547	2.137796			
qmof-e2e9e5f	-1.791733723	-5.867733723	4.076			
qmof-f848e64	-1.753919313	-6.075411313	4.321492			
qmof-89fb1f3	-3.418300218	-5.963088218	2.544788			
qmof-05279d0	-2.373714643	-5.712576643	3.338862			
qmof-ad02239	-4.062462536	-6.099373536	2.036911			
qmof-6729ffe	-3.450337481	-5.708549481	2.258212	✓	✓	
qmof-e2e9016	-3.737984198	-5.623861198	1.885877			
qmof-7b0b569	-2.94384817	-6.03003417	3.086186			
qmof-5c0fddb	-2.766467651	-6.242760651	3.476293			
qmof-6da396d	-3.29502015	-5.83979315	2.544773			
qmof-1a90743	-2.646625439	-4.901999439	2.255374			
qmof-76ab95c	-3.319083178	-5.657292178	2.338209			
qmof-4b9ff08	-2.769690212	-5.053290212	2.2836			
qmof-3d4b29f	-2.889156097	-6.829264097	3.940108			
qmof-6585ef5	-3.235032358	-5.317516358	2.082484			
qmof-1072fba	-2.766312988	-5.701420988	2.935108			
qmof-1265040	-2.537452796	-5.327921796	2.790469			
qmof-002580c	-2.204496834	-6.284087834	4.079591			
qmof-7c5f404	-3.10024107	-6.71609607	3.615855			
qmof-7bcba44	-3.052387216	-6.829328216	3.776941			
qmof-afb7457	-3.953684679	-6.218853679	2.265169			
qmof-0505344	-3.821694657	-6.217864657	2.39617			

Continued on next page

Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-c605c0a	-2.236926394	-5.942531394	3.705605			
qmof-4dbdf12	-4.142416257	-6.867834257	2.725418			
qmof-7df997f	-2.887502008	-6.004342008	3.11684			
qmof-83de5c7	-3.763588757	-6.399250757	2.635662			
qmof-8fa9c85	-1.91203999	-6.06779599	4.155756			
qmof-f441841	-2.663482984	-6.466130984	3.802648			
qmof-a715883	-4.23197558	-8.37886158	4.146886			
qmof-b2a8e0e	-2.692847521	-6.817988521	4.125141			
qmof-dd76d21	-3.253006308	-6.874782308	3.621776			
qmof-45649ec	-2.858426443	-6.034963443	3.176537			
qmof-2943f96	-3.0748936	-7.0319446	3.957051			
qmof-be1b006	-3.577773231	-7.380694231	3.802921			
qmof-b89c781	-3.056228253	-5.979075253	2.922847			
qmof-2bb9974	-4.653609721	-6.771648721	2.118039			
qmof-be2d371	-3.264405716	-5.602094716	2.337689			
qmof-e4633f0	-4.264343396	-6.694252396	2.429909			
qmof-6815e74	-2.655830384	-4.841303384	2.185473			
qmof-ab89669	-2.793358536	-4.978896536	2.185538			
qmof-d42765b	-2.833909043	-6.036064043	3.202155			
qmof-bd41929	-3.140373273	-6.748519273	3.608146			
qmof-cff9a36	-1.964783515	-5.809407515	3.844624			
qmof-e4f97d4	-3.37386548	-6.964183481	3.590318			
qmof-5a93d85	-3.372358391	-5.973096391	2.600738			
qmof-aa662d6	-3.248331914	-6.804394914	3.556063			
qmof-1b6c849	-3.557066167	-6.392035167	2.834969			
qmof-5947f65	-2.794626948	-5.388335948	2.593709			
qmof-899ea4d	-2.339713602	-6.259154602	3.919441			
qmof-c8f0292	-2.151203092	-5.731118092	3.579915			
qmof-c430d7c	-3.029305269	-6.148141269	3.118836			
qmof-04459f0	-3.361575027	-5.731551027	2.369976	✓	✓	✓
qmof-52cac05	-3.963447876	-5.904627876	1.94118			
qmof-1fe6988	-2.890718117	-6.659084117	3.768366			
qmof-ad06ef4	-3.207711562	-6.832124562	3.624413			
qmof-0cfad40	-2.744296097	-6.253319097	3.509023			
qmof-c7fd3ba	-2.654940284	-6.730189284	4.075249			
qmof-1fd65b5	-3.966434738	-5.776596738	1.810162			
qmof-ed9a745	-1.473497157	-4.859820157	3.386323			
qmof-bd93f70	-2.528492287	-5.954893287	3.426401			
qmof-0122bb1	-3.050147172	-4.258021172	1.207874			
qmof-3c5b84b	-2.853469515	-6.438646515	3.585177			
qmof-5cf14ed	-2.503540916	-6.299489916	3.795949			
qmof-8030fac	-3.134368897	-6.607084897	3.472716			
qmof-e7b6156	-3.224584659	-5.298405659	2.073821			
qmof-42b6f78	-3.375088847	-5.551548847	2.17646			
qmof-e2b0729	-4.002344375	-5.731986375	1.729642			
qmof-04b3678	-2.483874142	-6.116451142	3.632577			
qmof-324fde1	-3.384433834	-6.904280834	3.519847			

Continued on next page

Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-47eb3b5	-3.418697787	-6.183493787	2.764796			
qmof-2c7d021	-2.346446186	-6.318414186	3.971968			
qmof-fae8514	-1.728667491	-6.010395491	4.281728			
qmof-817fdc2	-2.348231606	-5.092711606	2.74448			
qmof-e986fdb	-2.175362295	-5.457060295	3.281698			
qmof-7e9d037	-3.644641529	-6.132887529	2.488246	✓	✓	
qmof-8c3c946	-2.51731638	-6.47642338	3.959107			
qmof-1fa8bff	-2.659658279	-6.038455279	3.378797			
qmof-86d21dc	-2.691050333	-6.220926333	3.529876			
qmof-4b4c416	-2.248223089	-4.205325089	1.957102			
qmof-a4ece54	-2.493607401	-4.842922401	2.349315			
qmof-55f4d83	-3.210436566	-7.220006566	4.00957			
qmof-8bc481b	-2.544086024	-6.609578024	4.065492			
qmof-24cd035	-3.398060995	-7.285583995	3.887523			
qmof-ef047dc	-2.565233477	-6.484978477	3.919745			
qmof-9aa7703	-2.407026606	-5.775028606	3.368002			
qmof-6842f7a	-3.546698036	-6.010734036	2.464036	✓	✓	
qmof-cebd596	-2.372942921	-6.913402921	4.54046			
qmof-6c0ffdd	-2.204527642	-5.098005642	2.893478			
qmof-3356268	-4.459695932	-7.324266932	2.864571			
qmof-dba834	-3.181136276	-5.898306276	2.71717			
qmof-46324de	-3.024976435	-6.859762435	3.834786			
qmof-6db07a6	-2.580100878	-4.720161878	2.140061			
qmof-fd0958d	-3.551685007	-7.315355007	3.76367			
qmof-727c9e2	-2.841755654	-6.947003654	4.105248			
qmof-3010cb1	-3.369680154	-5.610754154	2.241074			
qmof-e57e5bf	-3.948346069	-6.603924069	2.655578			
qmof-a342218	-4.424059242	-7.299853242	2.875794			
qmof-ed6a1d6	-4.507679788	-6.807395788	2.299716			
qmof-2bf6c21	-3.226382907	-5.233829907	2.007447			
qmof-c67339d	-4.343400951	-6.700300951	2.3569			
qmof-0fe96c4	-3.550267076	-5.633323076	2.083056			
qmof-d38bd9e	-4.841557341	-6.731643341	1.890086			
qmof-3168ba7	-3.245005967	-5.252676967	2.007671			
qmof-e9ceb52	-3.419398195	-5.317541195	1.898143			
qmof-cda8e7d	-3.705439867	-5.622900867	1.917461			
qmof-6bca146	-4.751356544	-7.561962544	2.810606			
qmof-72a3c74	-3.815145059	-6.332514059	2.517369			
qmof-dcf8019	-3.984111795	-6.047387795	2.063276			
qmof-270bfcd	-3.815131133	-6.387817133	2.572686			
qmof-ddab43b	-3.591997857	-5.370982857	1.778985			
qmof-861ea4a	-3.5609502	-5.6491592	2.088209			
qmof-2155e19	-2.872907875	-4.741662875	1.868755			
qmof-dc2dcc2	-3.204353169	-5.656456169	2.452103			
qmof-c650339	-3.708358821	-5.725450821	2.017092	✓		
qmof-df4f7aa	-2.547849787	-4.691857787	2.144008			
qmof-9be2d4c	-2.993220906	-5.047162906	2.053942			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-260d2c2	-3.886347881	-6.295482881	2.409135			
qmof-1c25053	-3.825407732	-6.012326732	2.186919			
qmof-ae3b943	-3.794534374	-5.916836374	2.122302			
qmof-0625810	-4.467437716	-6.793479716	2.326042			
qmof-0e27a4a	-3.588663231	-5.982988231	2.394325	✓	✓	
qmof-53530b6	-3.25650285	-5.59788985	2.341387			
qmof-8b79c84	-3.329771364	-5.700308364	2.370537	✓	✓	✓
qmof-541d78e	-3.033736926	-5.202284926	2.168548			
qmof-2ae9d62	-4.332701492	-7.491847492	3.159146			
qmof-41141ee	-4.138461378	-5.870313378	1.731852			
qmof-e3a2152	-4.414868726	-6.438202726	2.023334			
qmof-7f07a21	-4.530818683	-6.560313683	2.029495			
qmof-b1b05e2	-4.61713916	-7.21816416	2.601025			
qmof-08a6002	-4.794491931	-7.363355931	2.568864			
qmof-4bdce90	-3.660207136	-6.403966136	2.743759			
qmof-23d6bfc	-4.093048618	-6.430418618	2.33737			
qmof-c7fdbb6	-4.00527442	-6.60933242	2.604058			
qmof-809fc5e	-3.87361859	-6.25809259	2.384474			
qmof-b46b341	-4.050755227	-6.368794227	2.318039			
qmof-9d7aabd	-4.903923105	-4.985264105	0.081341			
qmof-126dd4e	-4.551795849	-6.569957849	2.018162			
qmof-061695a	-3.977109166	-6.960526166	2.983417			
qmof-7c271cd	-3.721532779	-6.848165779	3.126633			
qmof-21f0ad6	-4.04900233	-7.20552633	3.156524			
qmof-87274e3	-5.330261843	-7.226723843	1.896462			
qmof-5ea3d58	-4.778204864	-7.326877864	2.548673			
qmof-2a66aa3	-4.489646642	-7.160127642	2.670481			
qmof-bab1656	-3.711107597	-6.472666597	2.761559			
qmof-93bad37	-2.925293627	-4.990099627	2.064806			
qmof-1f248c3	-3.877376275	-6.035934275	2.158558			
qmof-063efc4	-3.537411823	-5.898816823	2.361405	✓	✓	
qmof-70c044b	-3.811263844	-6.066386844	2.255123			
qmof-158f8fd	-2.767667453	-4.997852453	2.230185			
qmof-8bfe542	-3.582981877	-5.985038877	2.402057	✓	✓	
qmof-b8e941c	-4.159551251	-6.807906251	2.648355			
qmof-0cb7c52	-3.955983844	-6.546781844	2.590798			
qmof-c1bc002	-2.769179005	-4.933137005	2.163958			
qmof-1f7e34d	-2.999195732	-5.308537733	2.309342			
qmof-83816cc	-4.043321229	-6.187770229	2.144449			
qmof-15ff994	-3.750361539	-6.541617539	2.791256			
qmof-1ca8fd0	-3.973945129	-6.901710129	2.927765			
qmof-058b1bf	-3.82811494	-6.17111394	2.342999			
qmof-b58e86f	-3.883542082	-6.333216082	2.449674			
qmof-201a359	-2.897638833	-5.330695833	2.433057			
qmof-517524d	-3.908882806	-6.581725806	2.672843			
qmof-cf29560	-4.495771941	-6.843390941	2.347619			
qmof-540f79a	-4.419524576	-7.092460576	2.672936			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-47efcfb	-3.818073299	-6.557577299	2.739504			
qmof-9c92284	-4.432592892	-6.763045892	2.330453			
qmof-add590e	-3.887729722	-5.684855722	1.797126			
qmof-0749ed8	-3.984158251	-6.371016251	2.386858			
qmof-60ca16f	-4.165653546	-6.303727546	2.138074			
qmof-33426df	-3.821248549	-5.919043549	2.097795			
qmof-761ed66	-4.234220122	-6.216752122	1.982532			
qmof-17a96f5	-2.738989484	-4.872562484	2.133573			
qmof-1033c27	-3.054813044	-5.516780044	2.461967			
qmof-7705722	-4.876277307	-6.917477307	2.0412			
qmof-78cbecc	-5.314712763	-7.853172763	2.53846			
qmof-d32c5b6	-3.902443172	-6.537641172	2.635198			
qmof-e09709f	-3.26512454	-6.14514254	2.880018			
qmof-5e49283	-4.087380205	-6.628762205	2.541382			
qmof-a74572e	-4.541710882	-6.917550882	2.37584			
qmof-781949d	-3.66659981	-6.20147981	2.53488			
qmof-d4963a6	-4.188622749	-6.681025749	2.492403			
qmof-e58468d	-4.662245695	-6.684299695	2.022054			
qmof-0fb4c2f	-4.409681559	-6.432412559	2.022731			
qmof-051793e	-3.704802334	-5.676463334	1.971661	✓		
qmof-d844aae	-3.611947	-5.89535	2.283403	✓	✓	
qmof-97bca44	-3.282719657	-5.247375657	1.964656			
qmof-40fadd9	-3.486913291	-5.633408291	2.146495			
qmof-2b1d7b8	-3.459304784	-5.225299784	1.765995			
qmof-74256d1	-4.235969536	-6.484432536	2.248463			
qmof-288d36e	-4.290011963	-6.872338963	2.582327			
qmof-87b704c	-4.447092479	-6.483940479	2.036848			
qmof-b4a9394	-3.326943605	-5.495033605	2.16809			
qmof-69e96ed	-3.733756507	-6.283151507	2.549395			
qmof-4b9332b	-4.002747804	-5.764496804	1.761749			
qmof-1bdd4c5	-2.775010106	-4.873816106	2.098806			
qmof-d74c3da	-4.59411432	-6.79726232	2.203148			
qmof-3aa5315	-4.379430065	-6.322246065	1.942816			
qmof-e17884e	-3.739483642	-5.907401642	2.167918	✓		
qmof-5964493	-3.826235639	-5.720017639	1.893782			
qmof-56a4d8e	-4.629714868	-6.471187868	1.841473			
qmof-4c6786c	-3.07935368	-5.20463968	2.125286			
qmof-e65b4c0	-3.803938414	-6.058175414	2.254237			
qmof-35465ea	-2.805499521	-4.963421521	2.157922			
qmof-006f9b7	-3.848145583	-5.861136583	2.012991			
qmof-bc956a0	-3.802223241	-5.941956241	2.139733			
qmof-0c697c4	-3.955020031	-6.171896031	2.216876			
qmof-2446a3a	-3.353224037	-5.731132037	2.377908	✓	✓	✓
qmof-ddbf934	-4.390678679	-6.128795679	1.738117			
qmof-79de66a	-2.982839256	-4.925731256	1.942892			
qmof-68146ae	-3.313038788	-5.242450788	1.929412			
qmof-7d8b8c4	-5.032919899	-7.048814899	2.015895			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-db703b3	-4.323162348	-6.291818348	1.968656			
qmof-2246e1d	-3.970241291	-5.523201291	1.55296			
qmof-40c4e6c	-3.734484907	-5.616915907	1.882431			
qmof-16edcac	-4.424344241	-6.314333241	1.889989			
qmof-51350de	-4.027731911	-6.030598911	2.002867			
qmof-40f78ce	-4.301947579	-6.278847579	1.9769			
qmof-76e7dc6	-2.793601864	-4.919680864	2.126079			
qmof-2e34efd	-4.09178006	-6.08905306	1.997273			
qmof-029d2b0	-3.193889982	-5.316261982	2.122372			
qmof-abd1ccd	-4.167140707	-5.813041707	1.645901			
qmof-304d957	-4.035900912	-5.707750912	1.67185			
qmof-3eac45e	-4.085829245	-5.762510246	1.676681			
qmof-d68f170	-3.940360673	-5.534594673	1.594234			
qmof-3ef068e	-4.205065856	-5.886122856	1.681057			
qmof-e7b4875	-3.153432688	-5.050150688	1.896718			
qmof-79f0214	-3.053805513	-5.209961513	2.156156			
qmof-ba67bb7	-2.427129247	-4.664338247	2.237209			
qmof-87276cb	-3.61756522	-5.44887422	1.831309			
qmof-e252678	-3.379078818	-5.458268818	2.07919			
qmof-d4c0a72	-3.059879932	-5.231854932	2.171975			
qmof-44399ca	-3.375662924	-5.654703924	2.279041			
qmof-4615dbd	-4.735812485	-6.882399485	2.146587			
qmof-aab2608	-4.145226372	-6.035049372	1.889823			
qmof-8d68d51	-4.347503187	-6.282416187	1.934913			
qmof-c6cc493	-3.155504715	-5.484065715	2.328561			
qmof-8f0fcd4	-4.717485272	-7.186489272	2.469004			
qmof-33c6e83	-3.18436566	-5.582348661	2.397983			
qmof-909d17d	-3.975060596	-6.361406596	2.386346			
qmof-a5c7ba1	-4.089852879	-6.140773879	2.050921			
qmof-0ad522b	-3.460309234	-6.450516234	2.990207			
qmof-e2c816e	-4.88953495	-7.28628295	2.396748			
qmof-d480554	-4.362346086	-6.315731086	1.953385			
qmof-38c74f5	-4.412738471	-6.488574471	2.075836			
qmof-94af341	-4.497862466	-6.542196466	2.044334			
qmof-555bacb	-4.918684211	-7.830678211	2.911994			
qmof-dda1cb2	-3.792445911	-5.998472911	2.206027			
qmof-b8f1825	-4.833213926	-7.864266926	3.031053			
qmof-6c81e33	-3.555711552	-5.795894552	2.240183	✓	✓	
qmof-1ca5878	-3.917533928	-5.970141928	2.052608			
qmof-ad7ba6d	-3.714803334	-6.656495334	2.941692			
qmof-670fdd3	-4.622732232	-6.844754232	2.222022			
qmof-0daa435	-6.175010164	-8.077648164	1.902638			
qmof-4f0af97	-4.633384957	-6.595396957	1.962012			
qmof-4048940	-4.126259477	-6.447719477	2.32146			
qmof-6ebc141	-3.557791775	-6.124106775	2.566315			
qmof-33b0cbe	-3.864805234	-6.502943234	2.638138			
qmof-0b51679	-3.937505516	-5.881386516	1.943881			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-7a13182	-3.524410753	-5.564311753	2.039901			
qmof-23c88cb	-2.366108496	-4.808868496	2.44276			
qmof-764dc05	-3.000038471	-5.221067471	2.221029			
qmof-abb0c43	-2.691977658	-4.678478657	1.986501			
qmof-3620829	-3.065544265	-5.336793265	2.271249			
qmof-08a8daa	-5.106712537	-7.066855537	1.960143			
qmof-8797c78	-3.844732105	-5.645084105	1.800352			
qmof-649b3f2	-2.318252245	-4.313954245	1.995702			
qmof-3467823	-2.249467959	-4.303677959	2.05421			
qmof-a1c8920	-2.952248743	-4.818754743	1.866506			
qmof-09ba5e4	-5.59398778	-7.47028478	1.876297			
qmof-2e1f180	-4.813581587	-6.906081587	2.0925			
qmof-6bab288	-3.466257021	-5.566631021	2.100374			
qmof-7d881b1	-5.102876658	-7.149349658	2.046473			
qmof-645a178	-4.573064075	-6.532161075	1.959097			
qmof-27e2c83	-3.878870956	-6.144912956	2.266042			
qmof-0b496b6	-4.47024568	-7.00949768	2.539252			
qmof-24e85d6	-4.87772644	-7.12949744	2.251771			
qmof-f07e952	-5.316312571	-7.356388571	2.040076			
qmof-edc50fe	-4.09748293	-6.76483393	2.667351			
qmof-be35ab2	-4.073762057	-6.650895057	2.577133			
qmof-6efed02	-4.084632253	-6.256566253	2.171934			
qmof-b5a79ba	-4.007293002	-6.326817002	2.319524			
qmof-80c10f6	-5.067096375	-7.414222376	2.347126			
qmof-8c5d275	-4.342200916	-6.828315916	2.486115			
qmof-b4a544a	-4.627790621	-6.718782621	2.090992			
qmof-d2f08f6	-3.911419508	-6.000567508	2.089148			
qmof-57e937f	-4.200270812	-6.135114812	1.934844			
qmof-f19d234	-3.897383486	-5.976381486	2.078998			
qmof-a567c29	-4.618472123	-6.811222123	2.19275			
qmof-6f89314	-4.361711691	-6.915250691	2.553539			
qmof-231ce7d	-3.783327665	-5.206413665	1.423086			
qmof-878fcc2	-4.381677392	-5.737490392	1.355813			
qmof-d15583a	-4.281612639	-5.539899639	1.258287			
qmof-f05406c	-3.944470681	-6.060032681	2.115562			
qmof-a04209a	-4.176512993	-5.972881993	1.796369			
qmof-10cb6cd	-4.14441284	-6.12925584	1.984843			
qmof-1d7abc8	-4.359824473	-6.237578473	1.877754			
qmof-4a57b79	-4.420990853	-6.218005853	1.797015			
qmof-0e8c4b6	-4.120477912	-6.207689912	2.087212			
qmof-8bfc542	-4.425653621	-6.523182621	2.097529			
qmof-4ae6ad4	-3.835878044	-6.192044044	2.356166			
qmof-0d33b0c	-4.112742863	-6.266394863	2.153652			
qmof-d1061d7	-4.114225014	-6.225606014	2.111381			
qmof-e230445	-4.357574239	-6.141079239	1.783505			
qmof-8809609	-3.904908425	-5.779026425	1.874118			
qmof-ae6b8ab	-3.177053418	-5.280988418	2.103935			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-bea0429	-4.041161998	-6.349199998	2.308038			
qmof-2bdd6ef	-4.307764113	-6.255842113	1.948078			
qmof-3d670d8	-3.461770337	-5.319643337	1.857873			
qmof-b5c7314	-3.220919235	-5.456016235	2.235097			
qmof-0475987	-2.305424685	-4.427024685	2.1216			
qmof-9997f68	-3.681721301	-5.794253301	2.112532	✓		
qmof-9b52dea	-3.161190555	-5.096859555	1.935669			
qmof-25097fe	-4.72110866	-6.67868566	1.957577			
qmof-cec6153	-3.375148804	-5.675722804	2.300574	✓	✓	✓
qmof-4e884d7	-3.221671012	-5.186132012	1.964461			
qmof-7616aac	-4.053419359	-6.483462359	2.430043			
qmof-6ba8301	-4.905321361	-6.935046361	2.029725			
qmof-65ef97b	-3.530951632	-5.861308632	2.330357	✓	✓	
qmof-dabb11e	-3.905141957	-5.859435957	1.954294			
qmof-17a47b2	-2.615441709	-4.686009709	2.070568			
qmof-22f1463	-4.452201556	-5.032792556	0.580591			
qmof-29c0bd6	-4.274361339	-5.914719339	1.640358			
qmof-97d5d0e	-4.133126334	-5.799326334	1.6662			
qmof-825c2c6	-4.073114513	-5.855339513	1.782225			
qmof-8443b22	-4.411811186	-7.208904186	2.797093			
qmof-bbdb65b	-4.662856016	-6.606809016	1.943953			
qmof-d57448c	-3.957176641	-5.974477641	2.017301			
qmof-369262d	-4.478645548	-6.698552548	2.219907			
qmof-ddfc64a	-3.193066326	-4.784425326	1.591359			
qmof-9931f8f	-3.77239126	-6.03224426	2.259853	✓		
qmof-76de5fa	-4.165607366	-6.458885366	2.293278			
qmof-6a4cff2	-5.488325989	-8.233535989	2.74521			
qmof-eade42c	-4.388819244	-6.891721244	2.502902			
qmof-5ab6b28	-4.658220298	-7.203747298	2.545527			
qmof-070d551	-3.682472746	-6.220305746	2.537833			
qmof-49df74b	-3.924501941	-6.453949941	2.529448			
qmof-705b6ab	-3.805086937	-6.154780937	2.349694			
qmof-6038f07	-3.554048283	-6.232583283	2.678535			
qmof-e2185c7	-3.153307854	-5.125830854	1.972523			
qmof-8325046	-4.103356024	-5.969849024	1.866493			
qmof-250bcfe	-3.57446233	-6.02207533	2.447613	✓	✓	
qmof-3a9cbbf	-4.134925707	-6.923286707	2.788361			
qmof-1b6b7d3	-4.014529102	-6.610899102	2.59637			
qmof-d71e4e0	-4.045038411	-6.688014411	2.642976			
qmof-3c935c8	-3.738622775	-6.476034775	2.737412			
qmof-8b511ee	-4.540777668	-6.891672668	2.350895			
qmof-dc505ad	-3.590275913	-6.454009913	2.863734			
qmof-35e2d08	-3.602982639	-6.442778639	2.839796			
qmof-513e1bb	-3.379929944	-6.340541944	2.960612			
qmof-20529db	-3.98187127	-6.71439527	2.732524			
qmof-748e762	-3.534850237	-5.524023237	1.989173			
qmof-a6f3f87	-3.995716536	-5.987001536	1.991285			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-38471da	-3.671469465	-5.761464465	2.089995	✓		
qmof-0743acf	-4.457709942	-6.865275942	2.407566			
qmof-c85eddf	-4.137334688	-6.747963688	2.610629			
qmof-2e2ea03	-3.916205218	-6.583972219	2.667767			
qmof-22baac9	-4.078705059	-6.681250059	2.602545			
qmof-5b07106	-3.774279508	-5.956550508	2.182271	✓		
qmof-e5adf3c	-4.038787902	-6.778508902	2.739721			
qmof-ef72fd7	-4.022693121	-6.399234121	2.376541			
qmof-26920f5	-3.800123214	-6.265984214	2.465861			
qmof-0fa90ce	-4.686086199	-6.595047199	1.908961			
qmof-35e0b44	-3.638608495	-5.896287495	2.257679	✓	✓	
qmof-5a70274	-3.460776346	-6.574703346	3.113927			
qmof-e29169f	-3.882576704	-5.723265704	1.840689			
qmof-99e633f	-3.418387377	-5.425381377	2.006994			
qmof-0a7a2fd	-4.696432003	-6.378731003	1.682299			
qmof-3133b45	-3.041013277	-4.925088277	1.884075			
qmof-e1625e5	-3.67880942	-5.93099842	2.252189	✓		
qmof-2665f66	-3.416216289	-6.523615289	3.107399			
qmof-63e34f0	-3.765095211	-5.932594211	2.167499	✓		
qmof-bdc796a	-4.813794057	-6.872340057	2.058546			
qmof-2c46c8a	-3.707072519	-6.682544519	2.975472			
qmof-51a592d	-3.921959058	-5.866515058	1.944556			
qmof-7dbd529	-3.911720903	-6.503253903	2.591533			
qmof-34451ee	-3.411267632	-6.314190632	2.902923			
qmof-320bc35	-3.702791284	-5.953358284	2.250567	✓		
qmof-b7be715	-3.133569546	-5.944245546	2.810676			
qmof-ad4b0d7	-3.206038591	-5.382821591	2.176783			
qmof-1f8a415	-3.181947094	-5.100534094	1.918587			
qmof-d7e755d	-4.351080433	-6.411887433	2.060807			
qmof-ef93a15	-3.263008587	-5.436413587	2.173405			
qmof-d5b7dd9	-5.295131802	-7.272203802	1.977072			
qmof-c63d32a	-3.893761118	-5.965751118	2.07199			
qmof-d76ea7b	-3.231458698	-5.465907698	2.234449			
qmof-68d0826	-3.623748288	-5.865960288	2.242212	✓	✓	
qmof-994af66	-3.873663504	-6.041976504	2.168313			
qmof-48537be	-3.349345881	-5.723819881	2.374474	✓	✓	✓
qmof-508fdd0	-3.998388312	-6.351678312	2.35329			
qmof-14fcdee	-3.839486458	-5.618322458	1.778836			
qmof-02e17f1	-2.816656748	-4.789500748	1.972844			
qmof-8bfd99e	-4.222411093	-5.843356093	1.620945			
qmof-5e5ad16	-1.999076123	-4.389852123	2.390776			
qmof-7daffde	-2.645855498	-4.628832498	1.982977			
qmof-b867fda	-4.120150639	-5.938540639	1.81839			
qmof-36d73a2	-3.993205883	-5.785707883	1.792502			
qmof-85dd0ae	-4.051450108	-5.968179108	1.916729			
qmof-7974618	-3.510147832	-5.340659832	1.830512			
qmof-b0410f7	-2.547129908	-4.301007908	1.753878			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-df6a8cc	-3.338688675	-5.499132675	2.160444			
qmof-16937aa	-3.515347731	-5.599678731	2.084331			
qmof-cafa193	-3.713705893	-6.030851893	2.317146	✓		
qmof-9c61283	-3.922170094	-6.194083094	2.271913			
qmof-d5e77c0	-3.489799462	-5.688804462	2.199005	✓	✓	
qmof-affcedc	-3.988239263	-6.045179263	2.05694			
qmof-42a8827	-3.016033699	-5.225258699	2.209225			
qmof-1b3859b	-3.141295697	-5.299620697	2.158325			
qmof-178fc48	-2.642495484	-4.428497484	1.786002			
qmof-83d60f6	-3.943165684	-6.065319684	2.122154			
qmof-959fc3d	-3.416321351	-5.635881351	2.21956			
qmof-9c0ae5c	-4.045597338	-5.755184338	1.709587			
qmof-d535864	-3.723880524	-5.910801524	2.186921	✓		
qmof-57e829d	-2.666707129	-5.030648129	2.363941			
qmof-5ee8a95	-1.797758605	-5.922665605	4.124907			
qmof-e266949	-1.789930663	-5.885649663	4.095719			
qmof-e172a22	-2.922841168	-6.698164168	3.775323			
qmof-19ecdb0	-2.237445819	-5.663244819	3.425799			
qmof-df86412	-3.003899455	-5.477879455	2.47398			
qmof-be3ffea	-2.583796397	-6.095420397	3.511624			
qmof-7ce0736	-2.966818631	-6.612547631	3.645729			
qmof-0385604	-2.967306627	-7.249429628	4.282123			
qmof-4b1ef88	-1.786205872	-4.702070872	2.915865			
qmof-22ff87f	-2.752320537	-5.261624537	2.509304			
qmof-c861c48	-1.99641662	-4.722411621	2.725995			
qmof-b0402ac	-1.60579549	-4.302780491	2.696985			
qmof-a8ea913	-2.387177561	-5.151842561	2.764665			
qmof-08c5035	-3.168778461	-4.969832461	1.801054			
qmof-0b09ca3	-3.503030533	-5.327901533	1.824871			
qmof-cd0f38e	-3.081234236	-6.133445236	3.052211			
qmof-145a0bf	-2.712241411	-5.598768411	2.886527			
qmof-4e9c14b	-2.725222284	-5.204917284	2.479695			
qmof-5a2471d	-2.988504536	-5.582232536	2.593728			
qmof-767c706	-2.615608706	-6.763142706	4.147534			
qmof-ebf848f	-2.74377184	-6.31021984	3.566448			
qmof-529911c	-3.641207188	-5.957760188	2.316553	✓	✓	
qmof-2449d69	-2.785047111	-5.293766111	2.508719			
qmof-64ce5e9	-3.37465837	-5.34819237	1.973534			
qmof-3b0015d	-2.274141272	-6.628122272	4.353981			
qmof-494ec46	-2.524398257	-5.119956257	2.595558			
qmof-705ecf9	-2.435882246	-5.778344246	3.342462			
qmof-6bd80b9	-3.880518189	-7.020776189	3.140258			
qmof-3eec122	-3.647854477	-5.857037477	2.209183	✓	✓	
qmof-010c828	-3.100598163	-5.924973163	2.824375			
qmof-02d2885	-3.880159731	-5.807472731	1.927313			
qmof-81003ca	-3.70361146	-6.80950846	3.105897			
qmof-b190302	-2.511475197	-5.479679197	2.968204			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-2adaa4e	-2.450624459	-5.525177459	3.074553			
qmof-d724ac4	-2.85842981	-5.27203881	2.413609			
qmof-8b93db2	-3.174493442	-6.233844442	3.059351			
qmof-1f389ca	-3.560644703	-7.787833703	4.227189			
qmof-8045d77	-2.573472229	-6.431954229	3.858482			
qmof-1ef74a7	-3.462041943	-5.888380943	2.426339	✓	✓	
qmof-0d1ec57	-1.954331427	-5.654071427	3.69974			
qmof-c16648b	-3.174687107	-6.630203107	3.455516			
qmof-3d08513	-4.557470749	-7.473760749	2.91629			
qmof-e4b5afc	-2.583079929	-6.113466929	3.530387			
qmof-db10139	-3.059239054	-6.259770054	3.200531			
qmof-ad34906	-2.686293522	-6.254967522	3.568674			
qmof-cbad0dc	-2.312071603	-5.178499603	2.866428			
qmof-e436871	-3.369349796	-6.622309796	3.25296			
qmof-2edfe81	-2.89911239	-6.14628439	3.247172			
qmof-a1ad69d	-2.939332642	-6.610046642	3.670714			
qmof-0cad810	-3.448631546	-6.216890546	2.768259			
qmof-0162588	-3.647492969	-6.026447969	2.378955	✓	✓	
qmof-3dcb1ed	-4.076035697	-7.399549697	3.323514			
qmof-2d4f3d7	-3.036708235	-6.802849235	3.766141			
qmof-09230cc	-3.450491386	-7.055230386	3.604739			
qmof-6d32b28	-1.79704281	-5.20326881	3.406226			
qmof-633815b	-3.435200387	-5.766776387	2.331576	✓	✓	
qmof-0e16ae3	-2.760060066	-6.599936066	3.839876			
qmof-01aff47	-3.050582104	-6.656088104	3.605506			
qmof-0fbdbe2	-2.114966212	-5.952504212	3.837538			
qmof-26780e7	-2.890413483	-6.467311483	3.576898			
qmof-48d242f	-2.926892442	-6.553159442	3.626267			
qmof-88da678	-2.922670402	-5.746580402	2.82391			
qmof-f564469	-2.562554022	-6.565780022	4.003226			
qmof-f198a27	-4.021206342	-6.819426342	2.79822			
qmof-60ed3b0	-2.788884269	-6.781143269	3.992259			
qmof-f04f83a	-2.895460538	-7.054624538	4.159164			
qmof-e2db1dc	-3.572496108	-6.991201108	3.418705			
qmof-d5ed185	-2.391557049	-6.089272049	3.697715			
qmof-402c9c0	-4.101770732	-6.417206732	2.315436			
qmof-b5d33ff	-4.08154942	-6.70519142	2.623642			
qmof-1c69162	-4.540716233	-6.941983233	2.401267			
qmof-91b0193	-3.891968988	-5.456158988	1.56419			
qmof-b68a0ad	-2.993427004	-6.198666004	3.205239			
qmof-13889cb	-1.818503248	-4.742245248	2.923742			
qmof-23d6b4a	-4.961279877	-6.785487878	1.824208			
qmof-5113051	-3.835871558	-7.233787558	3.397916			
qmof-d76f8fd	-1.885559848	-5.272134848	3.386575			
qmof-9690414	-3.048229331	-6.233294331	3.185065			
qmof-a67dee3	-3.412448147	-7.075783147	3.663335			
qmof-3459f4d	-1.925125963	-5.991469963	4.066344			

Continued on next page

Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-511e8da	-1.929575556	-5.980845556	4.05127			
qmof-64fe339	-3.371289286	-6.492296286	3.121007			
qmof-b5a4fdc	-1.497798652	-5.606460652	4.108662			
qmof-6236874	-2.245689518	-5.721958518	3.476269			
qmof-80adb76	-3.806991416	-6.034827416	2.227836			
qmof-8d7621b	-2.263060944	-5.994822944	3.731762			
qmof-42e8bf9	-3.13185431	-5.97710731	2.845253			
qmof-1009afb	-3.759753765	-6.433371765	2.673618			
qmof-fbdc467	-2.980489364	-6.447673364	3.467184			
qmof-a4d16f2	-2.923447847	-6.821128847	3.897681			
qmof-05cc789	-2.171388618	-6.251512618	4.080124			
qmof-7901ba3	-3.289542836	-7.382732836	4.09319			
qmof-04bf78f	-2.645030394	-4.999219394	2.354189			
qmof-e8a6a82	-3.029209647	-5.362629647	2.33342			
qmof-3172fe0	-1.913564322	-5.488286322	3.574722			
qmof-f818993	-2.448004271	-5.338884271	2.89088			
qmof-37419af	-2.685470476	-5.710751476	3.025281			
qmof-a5a3523	-2.189644345	-6.294430345	4.104786			
qmof-db61142	-2.152583129	-6.247495129	4.094912			
qmof-1f95408	-4.769618545	-7.375783545	2.606165			
qmof-05f7938	-1.72267306	-5.18224306	3.45957			
qmof-76a0d99	-2.278798911	-5.715052911	3.436254			
qmof-7bfdb52	-1.929331385	-5.781383385	3.852052			
qmof-2d6d0e3	-3.489164876	-6.259986876	2.770822			
qmof-66c3285	-3.796576271	-6.166660271	2.370084			
qmof-437d9f5	-3.392524603	-7.356901603	3.964377			
qmof-35c161a	-3.75038523	-6.77332923	3.022944			
qmof-571d405	-4.692878494	-8.557051494	3.864173			
qmof-8281b85	-1.955087051	-4.661707051	2.70662			
qmof-38e0c3c	-2.311213485	-5.383199486	3.071986			
qmof-f26628c	-1.639386335	-5.690903335	4.051517			
qmof-71d890d	-3.587049899	-5.726546899	2.139497	✓	✓	
qmof-8b50b3f	-3.460159537	-6.316402537	2.856243			
qmof-5a28a47	-2.105596255	-6.143163255	4.037567			
qmof-a7b40bb	-3.369535716	-6.652654716	3.283119			
qmof-5d60ff1	-2.355985777	-4.779632777	2.423647			
qmof-eee201d	-4.296666602	-6.303841602	2.007175			
qmof-651a0e2	-4.127748982	-6.187336982	2.059588			
qmof-e581c0e	-3.756088563	-5.721753563	1.965665	✓		
qmof-2ad6ccc	-3.06989084	-5.97545084	2.90556			
qmof-d21a0d9	-4.085503102	-6.903974102	2.818471			
qmof-5108c60	-3.773616695	-6.009503695	2.235887	✓		
qmof-3be1907	-3.473824469	-6.936916469	3.463092			
qmof-94ab9a7	-3.029847056	-6.876967056	3.84712			
qmof-e62d92a	-3.805197193	-6.745308193	2.940111			
qmof-295bfb2	-3.162323433	-6.606916433	3.444593			
qmof-5c4ddd4	-3.41115796	-6.57541696	3.164259			

Continued on next page

Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-534ec49	-2.770840578	-5.860495579	3.089655			
qmof-3dfbcbcd	-3.434380043	-6.149744043	2.715364			
qmof-f67a0ff	-3.332842926	-6.432160926	3.099318			
qmof-b5b8b3e	-1.792105567	-5.412606567	3.620501			
qmof-ec8a9b7	-1.311534566	-4.505719566	3.194185			
qmof-308a75f	-1.866184198	-7.169453198	5.303269			
qmof-d47a2d7	-3.629759667	-5.919715667	2.289956	✓	✓	
qmof-2c0fa92	-2.56255227	-4.72917927	2.166627			
qmof-5206c61	-3.690092973	-6.878499973	3.188407			
qmof-5e2dc9c	-2.97301536	-6.51360736	3.540592			
qmof-206e25b	-2.70952591	-5.01009291	2.300567			
qmof-85fa9ba	-3.80500765	-6.56287065	2.757863			
qmof-09a1847	-3.888043503	-6.376964503	2.488921			
qmof-fee2e35	-3.377158592	-7.035053592	3.657895			
qmof-95786c6	-2.912630802	-6.798690802	3.88606			
qmof-720efb8	-2.673043761	-5.939261761	3.266218			
qmof-d6ddf36	-2.702859336	-6.181646336	3.478787			
qmof-5402e4d	-3.777055899	-7.826039899	4.048984			
qmof-27ecb45	-2.10279506	-5.31850606	3.215711			
qmof-70a1fa1	-3.188644644	-5.477987644	2.289343			
qmof-a077195	-2.600723641	-5.228864641	2.628141			
qmof-d4dbf80	-1.69005519	-5.12181719	3.431762			
qmof-749e21d	-3.10277344	-6.77447044	3.671697			
qmof-05d14ae	-3.814771724	-7.997104724	4.182333			
qmof-6400cd1	-2.722891914	-6.530404914	3.807513			
qmof-1e272e4	-2.926001952	-5.389038952	2.463037			
qmof-9fd6fe0	-2.954797031	-4.946058031	1.991261			
qmof-711c472	-3.809328612	-6.289684612	2.480356			
qmof-68f6f0b	-2.69142367	-6.67248867	3.981065			
qmof-ce1aea4	-2.874672064	-4.980570064	2.105898			
qmof-930ace4	-3.071414576	-6.481146577	3.409732			
qmof-3328a0c	-2.566067792	-5.587795792	3.021728			
qmof-10b84fb	-2.666404052	-6.353685052	3.687281			
qmof-76724f2	-2.573044088	-4.879732088	2.306688			
qmof-9ae4bed	-2.188798139	-5.980623139	3.791825			
qmof-54e279c	-2.421924125	-4.419479125	1.997555			
qmof-1e98fe6	-2.805166794	-6.645244794	3.840078			
qmof-77aef10	-3.857089276	-6.212120276	2.355031			
qmof-e987c82	-2.641316558	-4.969406558	2.32809			
qmof-bdde1f9	-3.944735678	-6.794581678	2.849846			
qmof-cad0a5d	-2.630426654	-4.864192654	2.233766			
qmof-3c5c124	-3.028447799	-6.151077799	3.12263			
qmof-beb45ec	-3.257474096	-5.215951096	1.958477			
qmof-9c78145	-1.408038806	-6.340854806	4.932816			
qmof-3c04d40	-2.881632547	-5.165150547	2.283518			
qmof-6b21d44	-3.553345182	-7.249267182	3.695922			
qmof-8491731	-3.089648913	-5.841828913	2.75218			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-3f6db6f	-2.282468808	-6.293553808	4.011085			
qmof-64f190e	-2.531260605	-5.883065605	3.351805			
qmof-d1ed4a4	-1.812545826	-5.671023826	3.858478			
qmof-f2717c4	-2.411773157	-5.599294157	3.187521			
qmof-f9b83bc	-2.509960831	-5.908144831	3.398184			
qmof-93ec4e0	-3.104794019	-6.341124019	3.23633			
qmof-9d71d13	-3.28302739	-6.63433239	3.351305			
qmof-9c8ecba	-2.897257701	-6.708216701	3.810959			
qmof-1c14e71	-2.703616694	-6.331786694	3.62817			
qmof-914130f	-2.402582418	-6.367903418	3.965321			
qmof-41aa483	-2.352134237	-6.454409237	4.102275			
qmof-40093f4	-2.630528239	-4.712552239	2.082024			
qmof-642b86d	-3.656069301	-5.691527301	2.035458	✓		
qmof-2dae2b6	-2.67376874	-6.67313574	3.999367			
qmof-bf979d0	-3.117864593	-7.395382593	4.277518			
qmof-173e029	-2.401786992	-6.691003992	4.289217			
qmof-31a720c	-3.450079529	-7.226781529	3.776702			
qmof-9c01853	-2.85616334	-6.93423034	4.078067			
qmof-36d19a8	-3.129800083	-6.712899083	3.583099			
qmof-87bcd8	-5.060149572	-8.109931572	3.049782			
qmof-7ae1c7d	-2.755542562	-5.211289562	2.455747			
qmof-c3ff310	-2.295339261	-5.751814261	3.456475			
qmof-a0be11a	-2.987156986	-6.971385986	3.984229			
qmof-44525cd	-2.639463365	-4.456946365	1.817483			
qmof-62c9574	-3.252349173	-6.240618173	2.988269			
qmof-ce2d153	-3.809280347	-7.816385347	4.007105			
qmof-f645d00	-3.761115033	-7.923453033	4.162338			
qmof-d6f338e	-4.414071617	-6.453839617	2.039768			
qmof-8f835a4	-3.127950029	-7.171373029	4.043423			
qmof-d0a1c03	-3.162215066	-7.206415066	4.0442			
qmof-75de2e0	-2.773313429	-6.708853429	3.93554			
qmof-3e7238d	-3.166464635	-7.206678635	4.040214			
qmof-c0f392b	-3.678465293	-6.155720293	2.477255	✓		
qmof-74b1a87	-4.279355414	-6.143404414	1.864049			
qmof-63f404f	-4.185761935	-6.673581935	2.48782			
qmof-de95770	-2.530866172	-5.697473172	3.166607			
qmof-59b7a9f	-2.763463695	-6.011992695	3.248529			
qmof-d15d784	-2.87588901	-5.56293701	2.687048			
qmof-23596df	-4.253167429	-6.831653429	2.578486			
qmof-116061c	-4.106043165	-6.236991165	2.130948			
qmof-03090a5	-3.017248578	-5.390929578	2.373681			
qmof-7e5c22f	-3.627771328	-6.265437328	2.637666			
qmof-0b6ef72	-3.189648602	-5.580783602	2.391135			
qmof-ec3c0e8	-2.281253549	-4.591176549	2.309923			
qmof-b0f5ecd	-1.863194473	-4.531383473	2.668189			
qmof-8a8d2e8	-2.752660973	-7.029218973	4.276558			
qmof-ecac71f	-2.697595765	-6.793863765	4.096268			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-c2a60c1	-2.792938168	-6.714851168	3.921913			
qmof-8ce3f11	-3.964415625	-5.936141625	1.971726			
qmof-104309e	-5.155979987	-8.049720987	2.893741			
qmof-c10e1fd	-3.340321393	-7.073073393	3.732752			
qmof-7b3d567	-3.921520168	-6.084014168	2.162494			
qmof-c6cd4fd	-2.302614915	-6.107416915	3.804802			
qmof-9fbe71b	-4.515259218	-6.676547218	2.161288			
qmof-71a0ea3	-3.535922302	-7.136509302	3.600587			
qmof-3b1c2bf	-3.156983046	-7.102103046	3.94512			
qmof-09cb4ce	-3.165868016	-7.109000016	3.943132			
qmof-4c15177	-3.308870006	-6.228458006	2.919588			
qmof-8b5bb88	-5.246622356	-6.108122356	0.8615			
qmof-ddec51e	-2.795875045	-6.542173045	3.746298			
qmof-d0bf550	-3.162145105	-5.876259105	2.714114			
qmof-e6fc101	-2.879787097	-7.192727097	4.31294			
qmof-aa12b02	-3.224809006	-6.022839006	2.79803			
qmof-857c2d1	-2.247039681	-6.122284681	3.875245			
qmof-1681ab3	-2.858495426	-6.798399426	3.939904			
qmof-eef9492	-4.320046276	-7.151727276	2.831681			
qmof-be643de	-2.845601679	-6.727115679	3.881514			
qmof-18925a4	-3.26624903	-6.19447703	2.928228			
qmof-c0d0be0	-3.561540881	-6.862242881	3.300702			
qmof-70b2910	-3.258878335	-5.369057335	2.110179			
qmof-b053c87	-2.858621209	-6.596879209	3.738258			
qmof-b9e9c9e	-3.234732196	-6.844619196	3.609887			
qmof-df90041	-2.025218514	-5.825482514	3.800264			
qmof-374a046	-2.50037958	-6.81219258	4.311813			
qmof-f9c3fbb	-2.610739394	-6.566942394	3.956203			
qmof-0f66a7d	-3.560088991	-5.813768991	2.25368	✓	✓	
qmof-3e210ac	-2.940809666	-5.903844666	2.963035			
qmof-b7479eb	-2.773283583	-6.029528583	3.256245			
qmof-3288dd3	-2.079872083	-6.144727083	4.064855			
qmof-762bfda	-1.926853197	-5.901198197	3.974345			
qmof-99503b5	-3.153218416	-5.599920416	2.446702			
qmof-56bffcf	-2.443805954	-5.916273954	3.472468			
qmof-ac0b22d	-3.758824861	-7.215451861	3.456627			
qmof-2f09f08	-2.302472772	-6.263820772	3.961348			
qmof-9f89994	-3.220065225	-5.551644225	2.331579			
qmof-d9c6d97	-2.464350055	-4.837041055	2.372691			
qmof-b01516c	-4.02367181	-7.72228881	3.698617			
qmof-d689f74	-3.124759303	-6.343295303	3.218536			
qmof-5500d18	-3.601887626	-6.692998626	3.091111			
qmof-e0cfb23	-2.518696663	-5.529954663	3.011258			
qmof-44435b0	-3.76605645	-7.13803445	3.371978			
qmof-2d1b778	-2.038409824	-5.122449824	3.08404			
qmof-6d69c36	-2.617420151	-5.686035151	3.068615			
qmof-0c10f91	-2.947360093	-6.766260093	3.8189			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-88d427b	-1.653344248	-6.547747248	4.894403			
qmof-e2af422	-2.854176484	-5.530616484	2.67644			
qmof-c376f20	-2.93375127	-5.99393427	3.060183			
qmof-e25f3a3	-3.091410223	-7.271756223	4.180346			
qmof-1750ab0	-2.789300906	-6.417609906	3.628309			
qmof-e49dfd4	-2.548348656	-4.788685656	2.240337			
qmof-4f9c014	-1.533583853	-5.564578853	4.030995			
qmof-d65a785	-1.939945277	-5.842931277	3.902986			
qmof-ca7241d	-1.824814892	-5.802658892	3.977844			
qmof-d655f8d	-1.817218115	-6.068705115	4.251487			
qmof-a7a93aa	-3.055668565	-6.495867565	3.440199			
qmof-089b013	-1.863789956	-6.104692956	4.240903			
qmof-57b6935	-2.591307373	-6.332661373	3.741354			
qmof-f66d709	-2.918594313	-6.245561313	3.326967			
qmof-7c0089b	-3.332273818	-6.452203818	3.11993			
qmof-d689892	-3.401535426	-5.898254426	2.496719	✓	✓	✓
qmof-9034501	-3.060705783	-6.933512783	3.872807			
qmof-ee1da8c	-2.690418797	-5.068381797	2.377963			
qmof-8ed0ec6	-2.751319174	-4.955954174	2.204635			
qmof-ef5cc84	-3.389858444	-5.463724444	2.073866			
qmof-06bc0e5	-1.895681333	-5.674332333	3.778651			
qmof-90c218f	-2.04396862	-6.63079762	4.586829			
qmof-671d1a2	-1.755440183	-5.669104183	3.913664			
qmof-7bfb29d	-3.371223869	-7.218083869	3.84686			
qmof-05305ab	-3.507454324	-5.764682324	2.257228	✓	✓	
qmof-a2987bf	-3.15858657	-6.10320057	2.944614			
qmof-ad015e6	-1.645372717	-6.555870717	4.910498			
qmof-09e67ae	-4.664155017	-7.282241017	2.618086			
qmof-1dc8075	-3.440152962	-5.650920962	2.210768			
qmof-7541f7a	-2.291443949	-6.67907895	4.387635			
qmof-e993e6b	-3.151590949	-6.754493949	3.602903			
qmof-d17a645	-3.159684646	-7.111970646	3.952286			
qmof-5f22410	-2.858496934	-6.141393934	3.282897			
qmof-905f6f5	-2.734175152	-5.171257152	2.437082			
qmof-e72c3e9	-1.450426384	-6.135418384	4.684992			
qmof-fd9d828	-2.343635667	-6.203909667	3.860274			
qmof-875b2e9	-3.95525121	-6.77165921	2.816408			
qmof-1302ca9	-3.327461203	-7.263664203	3.936203			
qmof-74ea819	-4.372489835	-6.678609835	2.30612			
qmof-742cbde	-3.035980715	-6.567152715	3.531172			
qmof-fc8a9d4	-3.254995635	-7.035836635	3.780841			
qmof-29e411b	-3.074092225	-6.433421225	3.359329			
qmof-8ffd817	-2.556608682	-5.508274682	2.951666			
qmof-41a421b	-2.815136188	-5.673261188	2.858125			
qmof-e2ef78a	-2.956209927	-5.208041927	2.251832			
qmof-10aa8d9	-3.277336089	-5.772303089	2.494967	✓	✓	✓
qmof-002a6da	-2.699394376	-6.493219376	3.793825			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-1985e04	-2.732204009	-5.706541009	2.974337			
qmof-21e5b1b	-2.632265573	-6.554343573	3.922078			
qmof-cdf0dd2	-3.907788197	-7.320034197	3.412246			
qmof-bc46dbc	-3.512762239	-6.162852239	2.65009			
qmof-cc1705b	-3.245853528	-7.245714528	3.999861			
qmof-8fd5f30	-2.970268962	-7.037085962	4.066817			
qmof-bd2004d	-3.949710718	-7.132879718	3.183169			
qmof-afcc0ad	-1.872638804	-4.873663805	3.001025			
qmof-ba95831	-2.941861385	-5.147527386	2.205666			
qmof-8533641	-2.82747034	-6.74368234	3.916212			
qmof-f09c00f	-1.635075789	-5.823011789	4.187936			
qmof-dbcf346	-2.907527345	-7.124452345	4.216925			
qmof-f391693	-2.308139595	-5.397856595	3.089717			
qmof-ef7a4cd	-3.700359629	-7.730546629	4.030187			
qmof-e97bef9	-1.92789891	-5.983714911	4.055816			
qmof-4454b13	-3.668865289	-6.402824289	2.733959			
qmof-ed950f0	-2.092111901	-6.835688901	4.743577			
qmof-ea9f5eb	-3.34827385	-5.28403085	1.935757			
qmof-408d287	-2.147715237	-5.599082237	3.451367			
qmof-3c23f8c	-3.764186989	-6.250929989	2.486743	✓		
qmof-26483dd	-2.16817764	-5.45505064	3.286873			
qmof-e44a050	-1.915041037	-5.693968037	3.778927			
qmof-c32a137	-3.683138572	-6.355426572	2.672288			
qmof-19caac2	-3.132529578	-6.755219578	3.62269			
qmof-b981b73	-1.620508585	-6.111264585	4.490756			
qmof-d851c65	-2.820270304	-5.780445304	2.960175			
qmof-35b83fb	-3.380409428	-6.083664428	2.703255			
qmof-34904e2	-4.171609011	-6.310920011	2.139311			
qmof-59a2ee1	-2.942701492	-5.768857492	2.826156			
qmof-194d013	-2.883481814	-5.301414814	2.417933			
qmof-221d349	-3.960213045	-6.765774045	2.805561			
qmof-9e477b5	-1.964488851	-4.574318851	2.60983			
qmof-22084e3	-3.746491018	-5.752508018	2.006017	✓		
qmof-c5457b7	-2.04176295	-5.09015795	3.048395			
qmof-d108947	-3.035599575	-6.920474575	3.884875			
qmof-5c15ba0	-2.846839967	-5.532561967	2.685722			
qmof-9c2bfdc	-2.177680773	-4.726372773	2.548692			
qmof-e7ec47b	-2.956312537	-6.815063537	3.858751			
qmof-b30a68e	-2.656917858	-5.339088858	2.682171			
qmof-d867a6e	-3.008416771	-6.404954771	3.396538			
qmof-e58cc9d	-2.402177411	-4.833309411	2.431132			
qmof-a498ebd	-4.421816872	-7.200348872	2.778532			
qmof-50b9f96	-3.119565377	-7.371403377	4.251838			
qmof-ec286a6	-3.892443256	-7.666797256	3.774354			
qmof-dc165ea	-2.151283315	-6.037216315	3.885933			
qmof-e125d99	-3.487389305	-6.234339305	2.74695			
qmof-b110f68	-2.81342104	-6.84241204	4.028991			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-e16328e	-4.261703986	-7.219516986	2.957813			
qmof-6a840fe	-2.463047556	-6.092156556	3.629109			
qmof-e45b793	-2.905503706	-6.115762706	3.210259			
qmof-b1156fe	-3.093249554	-7.010128554	3.916879			
qmof-3de2d70	-2.491515113	-4.993892113	2.502377			
qmof-c71dee9	-2.938053775	-4.934147775	1.996094			
qmof-0cbcc26	-1.599384699	-6.6615477	5.062163			
qmof-f8c1b29	-3.780578723	-6.861147723	3.080569			
qmof-ff169e1	-1.790670083	-6.030426083	4.239756			
qmof-9fb6152	-2.202432189	-6.480479189	4.278047			
qmof-1e0a9c9	-2.498998624	-6.286415624	3.787417			
qmof-715f306	-3.634795897	-6.043596897	2.408801	✓	✓	
qmof-ceef48c	-2.927380314	-5.747327314	2.819947			
qmof-dd74e9c	-1.64593305	-6.50385905	4.857926			
qmof-efaa9ca	-3.053214735	-7.250909735	4.197695			
qmof-1b07b31	-3.976330719	-6.035423719	2.059093			
qmof-8a4c3d2	-2.400811021	-6.454393021	4.053582			
qmof-3415203	-2.926963343	-6.675440343	3.748477			
qmof-ae58b33	-3.774680477	-7.552770477	3.77809			
qmof-a5b6ce8	-2.40618868	-6.46288668	4.056698			
qmof-1507a40	-3.255719508	-5.341424508	2.085705			
qmof-9be438c	-3.440413562	-5.340747562	1.900334			
qmof-36fc2b5	-3.32749338	-6.13820538	2.810712			
qmof-5a5686e	-2.753143137	-6.347368137	3.594225			
qmof-255b822	-2.479233206	-5.430836206	2.951603			
qmof-34515cf	-2.534049897	-4.923421897	2.389372			
qmof-6250e57	-2.532234341	-5.690258341	3.158024			
qmof-1ad729f	-3.957534228	-6.749591228	2.792057			
qmof-e9fbf5f	-3.219681444	-6.831946444	3.612265			
qmof-0ca8b3d	-2.693411125	-5.019955125	2.326544			
qmof-0fd78a4	-1.990293566	-5.910806566	3.920513			
qmof-dc0cbac	-2.969581959	-6.374635959	3.405054			
qmof-6683238	-2.205292701	-5.789927701	3.584635			
qmof-650269a	-3.474885166	-7.250678166	3.775793			
qmof-43f07bb	-3.748358653	-5.917699653	2.169341	✓		
qmof-3a1e0f0	-2.952855509	-5.853863509	2.901008			
qmof-0b83e38	-3.594862035	-5.830073035	2.235211	✓	✓	
qmof-129e045	-4.313476413	-7.529464413	3.215988			
qmof-4cc3c71	-2.205927114	-5.807364114	3.601437			
qmof-bf9ccaf	-3.119177199	-5.781800199	2.662623			
qmof-b56b577	-3.925641721	-5.782138721	1.856497			
qmof-050c6ef	-2.158184873	-4.171308873	2.013124			
qmof-a1d1c28	-2.837252965	-6.371526965	3.534274			
qmof-d9c2d65	-3.310972316	-6.039067316	2.728095			
qmof-785f2a9	-3.078808232	-6.925309232	3.846501			
qmof-6db0296	-1.849818891	-6.259163891	4.409345			
qmof-a0b1b43	-3.418441492	-6.661648492	3.243207			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-a4a4669	-2.600997916	-5.380661916	2.779664			
qmof-e0eb4a6	-2.482836724	-6.846955724	4.364119			
qmof-2f9cf3e	-3.66365491	-5.50041291	1.836758			
qmof-a6a8f49	-2.923512355	-5.057568355	2.134056			
qmof-1ca4ac2	-2.107982716	-5.000511716	2.892529			
qmof-b882056	-2.947150129	-4.954708129	2.007558			
qmof-d6b4784	-2.73687638	-5.78465838	3.047782			
qmof-df87a37	-2.984899886	-6.160553887	3.175654			
qmof-b155426	-1.920895322	-5.374439322	3.453544			
qmof-694ec8a	-3.279945432	-5.637209432	2.357264			
qmof-7955c68	-4.073594095	-6.750878095	2.677284			
qmof-d44c3fa	-2.2992815	-6.3161735	4.016892			
qmof-8c0809c	-4.175658785	-7.603483785	3.427825			
qmof-d4d3c5f	-4.143915987	-5.734086987	1.590171			
qmof-fdeb493	-2.785113165	-6.064705165	3.279592			
qmof-561b7f4	-2.570156587	-6.267245587	3.697089			
qmof-d544575	-2.75173464	-4.94631664	2.194582			
qmof-cdc5769	-3.603898079	-5.867437079	2.263539	✓	✓	
qmof-4b4837b	-3.807677838	-5.825765838	2.018088			
qmof-eecf04e	-3.511591179	-5.303088179	1.791497			
qmof-73d1377	-3.149175195	-5.329206195	2.180031			
qmof-0b9c9b5	-2.929178226	-4.823202226	1.894024			
qmof-2522b56	-2.746991198	-4.805915198	2.058924			
qmof-5689ec9	-3.532250543	-5.777544543	2.245294	✓	✓	
qmof-65cfa24	-4.129567343	-6.140031343	2.010464			
qmof-6dc78ec	-3.073982637	-5.158189637	2.084207			
qmof-26dc3b8	-3.330845241	-5.111959241	1.781114			
qmof-14a36ed	-4.243793099	-6.330280099	2.086487			
qmof-3a9ad54	-3.327433465	-5.476692465	2.149259			
qmof-13f8e19	-3.900046219	-5.766045219	1.865999			
qmof-cf68a4b	-3.748582413	-5.798056413	2.049474	✓		
qmof-e8ce4cf	-3.071937933	-5.011378933	1.939441			
qmof-75d2f5f	-3.433783084	-5.752709084	2.318926	✓	✓	
qmof-9ef6fed	-3.557836066	-5.794672066	2.236836	✓	✓	
qmof-4410553	-3.153161489	-4.998323489	1.845162			
qmof-9489acc	-3.78662007	-5.80254207	2.015922	✓		
qmof-7df7140	-4.071046958	-5.832801958	1.761755			
qmof-a77a87b	-2.241497002	-4.151022002	1.909525			
qmof-32894ad	-5.180572256	-7.990310256	2.809738			
qmof-b0b952a	-3.112553934	-4.968150934	1.855597			
qmof-a84f36c	-6.85087411	-9.58988811	2.739014			
qmof-6afa476	-4.42805604	-6.31732704	1.889271			
qmof-b8bda61	-2.51733657	-4.16953257	1.652196			
qmof-efedb54	-4.633996918	-6.555080918	1.921084			
qmof-1594a7d	-3.783565505	-5.757893505	1.974328	✓		
qmof-6ebfed4	-3.740992842	-5.400270842	1.659278			
qmof-bd7e56c	-2.307526829	-4.447394829	2.139868			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-bd5b750	-3.25607886	-6.59083186	3.334753			
qmof-08ad999	-3.189824137	-6.111805137	2.921981			
qmof-c8860bc	-3.712256974	-6.874500974	3.162244			
qmof-1cc6d2b	-3.034142868	-6.437210868	3.403068			
qmof-baa76cb	-3.633619915	-6.874351915	3.240732			
qmof-362bef5	-3.487888121	-6.794073121	3.306185			
qmof-b731939	-4.177759365	-7.448256365	3.270497			
qmof-be54856	-3.354502475	-6.853933475	3.499431			
qmof-0d2f6a6	-3.958804735	-7.574988735	3.616184			
qmof-7e9c77b	-2.434954943	-5.526500943	3.091546			
qmof-34bb4c6	-4.3550796	-7.8421056	3.487026			
qmof-7370962	-5.197652749	-8.471314749	3.273662			
qmof-2308de6	-3.310219227	-6.635782227	3.325563			
qmof-22c6575	-3.263949046	-6.514277046	3.250328			
qmof-1b3e3c5	-3.7556115	-7.2125715	3.45696			
qmof-71d1286	-4.331833273	-7.792007273	3.460174			
qmof-94df011	-3.124986661	-6.662004661	3.537018			
qmof-19172d5	-3.715451409	-7.247435409	3.531984			
qmof-12bffdb	-3.601935023	-7.294246023	3.692311			
qmof-05f5f6e	-3.664309558	-7.321183558	3.656874			
qmof-626963a	-3.088390068	-5.298858068	2.210468			
qmof-ae4bb38	-3.475301779	-5.448351779	1.97305			
qmof-3298011	-3.435493212	-5.529252212	2.093759			
qmof-2eb73bf	0.266510018	-1.871548982	2.138059			
qmof-5f8bb84	-3.85883426	-6.10887726	2.250043			
qmof-167de54	-2.100202413	-4.179198413	2.078996			
qmof-2a30c18	-3.514590954	-5.523845954	2.009255			
qmof-d4d4dbf	-6.32015915	-7.97737615	1.657217			
qmof-9085c0a	-3.781886156	-5.824432156	2.042546	✓		
qmof-eb5a6a0	-4.468899573	-6.572858573	2.103959			
qmof-2b95566	-3.158845592	-5.319403592	2.160558			
qmof-d441ad0	-4.494486037	-6.283890037	1.789404			
qmof-25b107a	-3.422342228	-5.443151228	2.020809			
qmof-8eb67f4	-3.355842444	-5.040183444	1.684341			
qmof-44fa197	-3.227508445	-4.712174445	1.484666			
qmof-d088bbe	-3.314627738	-5.339474738	2.024847			
qmof-951ed7a	-4.327235517	-6.381296517	2.054061			
qmof-80fed89	-4.204694475	-5.958739475	1.754045			
qmof-bc01827	-3.641096968	-5.271126968	1.63003			
qmof-167482e	-3.061573196	-4.681819196	1.620246			
qmof-d159ad9	-2.921953389	-4.599874389	1.677921			
qmof-b078db5	-3.155399929	-4.771937929	1.616538			
qmof-a7d7957	-3.790463982	-5.483297982	1.692834			
qmof-ee6222e	-4.129123791	-5.697224791	1.568101			
qmof-3abfd72	-3.217916743	-5.287151743	2.069235			
qmof-7998d02	-3.628710809	-5.852613809	2.223903	✓	✓	
qmof-d3fae93	-3.579891663	-5.403736663	1.823845			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-8e3629b	-4.141787952	-6.127928952	1.986141			
qmof-acf445e	-2.602576989	-4.668425989	2.065849			
qmof-4d635ee	-2.928485951	-4.966776951	2.038291			
qmof-7615abf	-4.307459544	-6.103851544	1.796392			
qmof-2473511	-3.901615927	-6.063678927	2.162063			
qmof-5c2af2c	-3.535401523	-5.571635523	2.036234			
qmof-258a220	-2.217066365	-4.068114365	1.851048			
qmof-94e212d	-3.509097104	-5.623728104	2.114631			
qmof-c8c0b58	-3.992064052	-6.068593052	2.076529			
qmof-27df637	-2.85181484	-4.82845184	1.976637			
qmof-bd66dee	-3.675245845	-5.825786845	2.150541	✓		
qmof-9b1866d	-3.040078186	-5.244970186	2.204892			
qmof-35c8beb	-3.334388411	-5.096825411	1.762437			
qmof-214a25c	-3.253413832	-5.168998832	1.915585			
qmof-09319e1	-3.259284617	-5.009587617	1.750303			
qmof-e34c36e	-3.277934622	-5.030475622	1.752541			
qmof-decfa9	-3.207125414	-4.984114414	1.776989			
qmof-431f8cc	-3.227504168	-4.984920168	1.757416			
qmof-7f11edf	-3.961851819	-4.800628819	0.838777			
qmof-d6239ff	-3.533051206	-5.637202206	2.104151			
qmof-e86fcce	-2.219296755	-4.224557755	2.005261			
qmof-1ff5688	-3.914288356	-6.119641356	2.205353			
qmof-6d62075	-3.738782965	-5.783364965	2.044582	✓		
qmof-6127dd2	-3.94911463	-5.77004363	1.820929			
qmof-7bb0742	-3.725071499	-6.028558499	2.303487	✓		
qmof-a3576ea	-4.441668571	-6.717483571	2.275815			
qmof-9f20c48	-4.088301807	-6.294542807	2.206241			
qmof-628ac43	-3.763472726	-6.036369726	2.272897	✓		
qmof-03b6f67	-4.002187838	-5.666542838	1.664355			
qmof-8f38e7a	-4.851509183	-6.847984183	1.996475			
qmof-bbf6020	-2.884366379	-4.995094379	2.110728			
qmof-2556db0	-3.796946509	-5.780391509	1.983445			
qmof-8fbcfd3	-4.793749848	-7.185224848	2.391475			
qmof-b2fa897	-5.095356249	-6.946520249	1.851164			
qmof-48a8af6	-4.866891661	-6.994644661	2.127753			
qmof-78c366c	-4.39500176	-6.53323276	2.138231			
qmof-477bf52	-3.98381128	-6.20632128	2.22251			
qmof-9576ffc	-4.343912216	-6.370750216	2.026838			
qmof-c7f2375	-4.362315879	-6.377913879	2.015598			
qmof-46f2ccb	-4.438887248	-5.005796248	0.566909			
qmof-0dc00e5	-3.444128146	-5.581100146	2.136972			
qmof-9fd01d7	-3.144056254	-4.970367254	1.826311			
qmof-77e8bf6	-3.602039945	-5.767855945	2.165816	✓	✓	
qmof-791707c	-3.425805572	-5.483366572	2.057561			
qmof-a960f82	-3.212436387	-5.495098387	2.282662			
qmof-93db7c2	-3.451979067	-5.518443067	2.066464			
qmof-25a03d3	-3.737313449	-5.963914449	2.226601	✓		

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-8529597	-4.28976074	-6.26910374	1.979343			
qmof-c8ae741	-3.887611319	-5.775098319	1.887487			
qmof-87f5303	-3.752156148	-5.835998148	2.083842	✓		
qmof-f1859dd	-3.660879251	-5.602959251	1.94208			
qmof-7ee5c89	-3.331207422	-5.183254422	1.852047			
qmof-46ac557	-4.161589381	-6.464918381	2.303329			
qmof-8146e49	-3.204627798	-5.555883798	2.351256			
qmof-6e482fb	-3.530389436	-5.522906436	1.992517			
qmof-d192e8d	-3.103665382	-5.094353382	1.990688			
qmof-bb51b6f	-4.266392818	-6.074119818	1.807727			
qmof-de5e312	-2.756407115	-4.772719115	2.016312			
qmof-c4714cc	-3.627869215	-5.715922215	2.088053	✓	✓	
qmof-bc8f74e	-3.272334717	-5.093312717	1.820978			
qmof-7277549	-4.028395285	-6.024276285	1.995881			
qmof-a3c0179	-4.359444691	-6.418277691	2.058833			
qmof-2cfb7a7	-3.590988669	-5.792608669	2.20162	✓	✓	
qmof-8549a5b	-3.925869545	-5.788055545	1.862186			
qmof-ad4a6de	-2.68949971	-4.76035471	2.070855			
qmof-f0008e4	-2.693975581	-4.662891581	1.968916			
qmof-ca7a99c	-3.576677465	-5.532492465	1.955815			
qmof-730a3ab	-3.279886393	-5.185780393	1.905894			
qmof-9adf032	-3.291335982	-5.097652982	1.806317			
qmof-0496546	-2.972536917	-5.041212917	2.068676			
qmof-8648a69	-3.976833888	-5.900712888	1.923879			
qmof-726ab18	-2.72511087	-6.31793587	3.592825			
qmof-aae4521	-3.209607449	-6.432143449	3.222536			
qmof-b5a7513	-2.978192804	-6.208146804	3.229954			
qmof-3e22e52	-3.438799123	-7.602951123	4.164152			
qmof-c28fec8	-1.774827785	-5.894094785	4.119267			
qmof-136fa43	-2.885195242	-6.918949242	4.033754			
qmof-af5c9df	-2.783087648	-6.201446648	3.418359			
qmof-7dcae20	-2.896480318	-6.621189318	3.724709			
qmof-a248a94	-2.56720002	-6.01304802	3.445848			
qmof-c6917b4	-2.546200899	-5.757079899	3.210879			
qmof-6fd66b2	-1.446689329	-5.469741329	4.023052			
qmof-b439f25	-2.956434733	-4.786994733	1.83056			
qmof-510e27f	-1.697268577	-5.748334577	4.051066			
qmof-e4c240e	-3.581581078	-6.956347078	3.374766			
qmof-8242b5b	-3.337081405	-5.450909405	2.113828			
qmof-a996d0c	-3.332038118	-7.606936118	4.274898			
qmof-3d811dc	-3.061357162	-6.913037162	3.85168			
qmof-a47217e	-4.077165349	-5.942420349	1.865255			
qmof-a23970b	-3.111529504	-6.793198504	3.681669			
qmof-9ef6119	-2.70162913	-5.451444131	2.749815			
qmof-7e5ffee	-1.828765572	-6.101926572	4.273161			
qmof-15fdf79	-2.937017298	-6.897131298	3.960114			
qmof-46ab5ba	-2.84042589	-6.98862389	4.148198			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-e6770f4	-4.465556287	-7.931373287	3.465817			
qmof-835ab05	-4.270344282	-7.460654282	3.19031			
qmof-7c33b5f	-2.864839528	-6.719238528	3.854399			
qmof-011c3e3	-2.680164172	-5.395876172	2.715712			
qmof-e268c52	-2.14276809	-6.02043809	3.87767			
qmof-067c272	-3.58494911	-6.71669211	3.131743			
qmof-eaa4006	-3.517789236	-6.655573236	3.137784			
qmof-99810c8	-3.06601643	-5.99774843	2.931732			
qmof-ae5b951	-2.391071092	-4.864047092	2.472976			
qmof-14291f8	-0.894555018	-5.269539018	4.374984			
qmof-02d6206	-3.241566026	-5.978360027	2.736794			
qmof-ccbc5fe	-2.552479819	-6.236029819	3.68355			
qmof-b92e7e5	-3.263083257	-6.372009257	3.108926			
qmof-808b97f	-3.683159764	-7.052918764	3.369759			
qmof-14733c4	-2.582032957	-6.455451957	3.873419			
qmof-e8f57aa	-2.89790939	-6.80330239	3.905393			
qmof-569fecc	-3.242160313	-6.858506313	3.616346			
qmof-3d489e4	-3.343845341	-5.348770341	2.004925			
qmof-e5198b3	-2.690501515	-6.696389515	4.005888			
qmof-87d4896	-3.513671967	-6.364038967	2.850367			
qmof-d5c113e	-3.739901135	-6.550900135	2.810999			
qmof-77e8a1f	-3.323107136	-6.965633136	3.642526			
qmof-2f1a847	-2.43539302	-5.69320702	3.257814			
qmof-9b0bbdf	-2.97383433	-6.72228433	3.74845			
qmof-5a8d3cc	-2.667869881	-6.877781881	4.209912			
qmof-1eebafa	-3.251426144	-5.592480144	2.341054			
qmof-7375a78	-3.076603901	-6.241453901	3.16485			
qmof-938e4e7	-3.220449292	-6.138863292	2.918414			
qmof-15486a3	-2.609608114	-4.977641114	2.368033			
qmof-ae979f1	-2.738979316	-5.405013316	2.666034			
qmof-5f9a1bc	-2.740657758	-5.663755758	2.923098			
qmof-4f49da6	-2.549480824	-6.574396824	4.024916			
qmof-42b8b59	-2.919920463	-5.797966463	2.878046			
qmof-ab2c780	-3.802946718	-6.481007718	2.678061			
qmof-ed94e56	-3.235750336	-5.664885336	2.429135			
qmof-93977b0	-3.225850375	-6.787489375	3.561639			
qmof-108b337	-2.50072183	-6.31199383	3.811272			
qmof-9dce9f9	-2.228890181	-5.521301181	3.292411			
qmof-29090e7	-2.417506012	-5.934670012	3.517164			
qmof-35562f1	-2.230969725	-5.476215725	3.245246			
qmof-53516e2	-3.786943724	-7.846472724	4.059529			
qmof-14b170b	-1.88598226	-5.54354726	3.657565			
qmof-5dfdc69	-2.786130784	-6.759394784	3.973264			
qmof-73aa17b	-3.123384361	-6.490829361	3.367445			
qmof-c4c5c23	-2.420034733	-5.995068733	3.575034			
qmof-b874271	-4.593840111	-6.483460111	1.88962			
qmof-cfc442e	-2.444685838	-5.211504838	2.766819			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-2dc3acb	-2.853685948	-2.982088948	0.128403			
qmof-94e2360	-3.1253226	-5.7381316	2.612809			
qmof-a5caf55	-3.347829138	-7.054641138	3.706812			
qmof-95ef7fc	-3.277639471	-6.599712471	3.322073			
qmof-a4214c3	-2.65247365	-4.87579265	2.223319			
qmof-83c480c	-3.005994489	-5.522006489	2.516012			
qmof-e0ed021	-4.064307313	-7.418957313	3.35465			
qmof-2b1aba1	-2.468667859	-5.061916859	2.593249			
qmof-a4541ac	-2.918254307	-5.434460307	2.516206			
qmof-bd9a33a	-2.824278188	-5.356618188	2.53234			
qmof-a918c8a	-3.44926212	-6.15093312	2.701671			
qmof-7015fdd	-3.449034461	-6.163294461	2.71426			
qmof-e0cb981	-3.433851101	-6.132823101	2.698972			
qmof-c946ba5	-2.701631729	-4.894284729	2.192653			
qmof-beeff21	-3.950334841	-6.136130841	2.185796			
qmof-d5c670c	-3.241977524	-7.088245524	3.846268			
qmof-547262c	-3.110221892	-6.680917892	3.570696			
qmof-459525d	-3.894501936	-6.178873936	2.284372			
qmof-f1d2550	-3.381434536	-7.257914536	3.87648			
qmof-55ae928	-2.17486934	-6.25018234	4.075313			
qmof-648d493	-2.148758548	-6.245509548	4.096751			
qmof-17e43c6	-2.142280557	-6.239727557	4.097447			
qmof-55c6596	-2.583594469	-5.014804469	2.43121			
qmof-51ef3ab	-3.25183588	-5.51424788	2.262412			
qmof-73c6760	-1.116653846	-5.608736846	4.492083			
qmof-6812d65	-3.322675221	-6.842166221	3.519491			
qmof-7245894	-3.352719724	-6.827634724	3.474915			
qmof-32f203f	-3.454408332	-6.580959332	3.126551			
qmof-652d6b7	-3.430644866	-6.555382866	3.124738			
qmof-c585aa5	-4.165114701	-7.912202701	3.747088			
qmof-3bb4061	-3.218231062	-7.014746062	3.796515			
qmof-061fb4f	-3.462189333	-6.888452333	3.426263			
qmof-3f72d8d	-3.429530736	-5.511027736	2.081497			
qmof-51faf5d	-4.051684098	-6.852123098	2.800439			
qmof-76d9b07	-2.351461056	-4.983871056	2.63241			
qmof-c0bb078	-2.980575462	-6.499709462	3.519134			
qmof-a4420e2	-3.568468869	-7.318017869	3.749549			
qmof-b65c1f5	-3.352286428	-7.045476428	3.69319			
qmof-111ce53	-4.131603396	-6.812895396	2.681292			
qmof-9a7a487	-3.808820919	-7.764358919	3.955538			
qmof-2c4e323	-3.724088503	-7.736939503	4.012851			
qmof-a65e183	-3.748532137	-7.712059137	3.963527			
qmof-15285c1	-3.444061533	-6.965059533	3.520998			
qmof-e48a7ff	-2.691411097	-4.951339097	2.259928			
qmof-5cbefb9	-2.872886731	-5.921003731	3.048117			
qmof-859616a	-2.524024041	-6.052873041	3.528849			
qmof-f2e16cf	-3.124342856	-6.581778856	3.457436			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-77765c8	-2.494697188	-6.546045188	4.051348	✓	✓	
qmof-69ba10c	-3.635374882	-5.955270882	2.319896			
qmof-d2eb739	-2.642256386	-6.019444386	3.377188			
qmof-3f16763	-2.391230751	-5.563506751	3.172276			
qmof-9ed183c	-2.826492068	-6.403029068	3.576537			
qmof-919ea19	-1.78428177	-5.06274277	3.278461			
qmof-7ac41d1	-3.347643243	-5.908409243	2.560766			
qmof-ec02694	-2.839727862	-5.147976862	2.308249			
qmof-350f7da	-2.746448195	-4.529724195	1.783276			
qmof-9bc797a	-3.282594221	-6.592758221	3.310164			
qmof-8f1ddfa	-2.501459698	-6.368557698	3.867098			
qmof-d967b7b	-2.257615304	-6.346752304	4.089137			
qmof-1a5f96c	-7.908802057	-7.935955057	0.027153			
qmof-a770d67	-2.943045343	-7.090997343	4.147952			
qmof-9c977f5	-2.995078002	-7.124299002	4.129221			
qmof-0300d77	-2.981845614	-7.107459614	4.125614			
qmof-7bea0fe	-1.797125371	-5.684882371	3.887757			
qmof-5250d6e	-1.563119039	-6.061920039	4.498801			
qmof-b1d7587	-0.806063201	-6.241992201	5.435929			
qmof-91e9d17	-2.838664094	-6.290097094	3.451433			
qmof-32cb456	-3.174146449	-6.169664449	2.995518			
qmof-3f821f2	-3.256559434	-6.829456434	3.572897			
qmof-ac38828	-2.862535273	-5.226630273	2.364095			
qmof-13dcf5f	-3.050389136	-6.116907136	3.066518			
qmof-d29181f	-2.873204594	-6.057390594	3.184186			
qmof-57bd41b	-2.497957744	-5.350774744	2.852817			
qmof-20020d6	-4.030135553	-6.396350553	2.366215			
qmof-401de6d	-2.812320109	-5.489847109	2.677527			
qmof-1647c66	-2.464992164	-5.687532164	3.22254			
qmof-ae8c853	-2.773682084	-6.593715084	3.820033			
qmof-82e3584	-2.587094459	-5.951771459	3.364677			
qmof-a9002ca	-1.449341713	-5.490244713	4.040903			
qmof-e566fbb	-3.250578652	-6.198883652	2.948305			
qmof-7a117a2	-1.99352769	-5.93162169	3.938094			
qmof-69186ff	-1.971975855	-5.472877855	3.500902			
qmof-6898ab9	-2.402786388	-5.661420388	3.258634			
qmof-25e44c3	-3.678622339	-7.283368339	3.604746			
qmof-0df8088	-3.314315696	-6.665608696	3.351293			
qmof-d21e6d3	-3.694209445	-6.435085445	2.740876			
qmof-69fcbdc	-3.912157478	-6.661506478	2.749349			
qmof-190750b	-2.861682543	-6.715567543	3.853885			
qmof-d01663e	-2.836608261	-6.777051261	3.940443			
qmof-ba7c077	-3.875906889	-5.769214889	1.893308			
qmof-4a5ca9f	-1.545178342	-5.738151342	4.192973			
qmof-b3d9e07	-3.963610848	-6.968923848	3.005313			
qmof-993b30b	-1.426779347	-5.561130347	4.134351			
qmof-6694295	-2.543026368	-5.881323368	3.338297			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-8d2aecd	-2.279074759	-5.857108759	3.578034			
qmof-7185c72	-2.025731104	-5.134028104	3.108297			
qmof-1197fef	-1.980044203	-6.058347203	4.078303			
qmof-e9437e6	-2.788135122	-5.582825122	2.79469			
qmof-b5c2834	-2.563991771	-6.898402771	4.334411			
qmof-0d326c4	-2.993600734	-6.224995734	3.231395			
qmof-0d0bec4	-2.954194249	-5.699729249	2.745535			
qmof-efdc343	-2.864302786	-6.513364786	3.649062			
qmof-585e841	-2.817028894	-6.558953894	3.741925			
qmof-1b23ab1	-2.582508961	-6.304557961	3.722049			
qmof-0be7420	-3.109708097	-5.119309097	2.009601			
qmof-7ac9c16	-3.056119763	-5.094263763	2.038144			
qmof-7c74ed0	-3.045636975	-5.092304975	2.046668			
qmof-52e1c67	-3.048606137	-5.096688137	2.048082			
qmof-5b945c8	-3.043745125	-5.080390125	2.036645			
qmof-cfee5a8	-2.699638091	-6.544091091	3.844453			
qmof-a41b944	-3.042000619	-5.084050619	2.04205			
qmof-b5fc9ed	-4.665146323	-7.482590323	2.817444			
qmof-ab60730	-3.614501456	-6.188887456	2.574386			
qmof-a90117c	-2.825600578	-5.580807578	2.755207			
qmof-2521623	-3.520098851	-7.157086851	3.636988			
qmof-663ff1d	-2.470087879	-4.881770879	2.411683			
qmof-d4c1cf1	-2.631102953	-4.995591953	2.364489			
qmof-893d0b0	-3.54046035	-7.19757135	3.657111			
qmof-421c2b7	-2.4615771	-4.939344101	2.477767			
qmof-d6d1915	-2.803167401	-6.324152401	3.520985			
qmof-285da54	-1.192608577	-6.026053577	4.833445			
qmof-01cfceb	-2.38235802	-6.02462502	3.642267			
qmof-d698e20	-1.910556769	-5.474057769	3.563501			
qmof-b7f8729	-2.863790016	-5.901930016	3.03814			
qmof-2e6cac6	-3.595381888	-6.293209888	2.697828			
qmof-ab4fc49	-2.464461042	-5.656413042	3.191952			
qmof-bbecd43	-2.749649907	-6.450483907	3.700834			
qmof-dba9b91	-3.486543411	-6.256821411	2.770278			
qmof-d46593c	-2.039708999	-4.423761999	2.384053			
qmof-e8d1a8e	-2.659926488	-5.167376488	2.50745			
qmof-e482ff6	-2.717728054	-6.059224054	3.341496			
qmof-f16186c	-3.217628154	-6.106168154	2.88854			
qmof-b265206	-3.390158816	-6.350458816	2.9603			
qmof-955f74a	-2.888950721	-5.251453722	2.362503			
qmof-ed04df4	-2.925400665	-6.925813665	4.000413			
qmof-b1a98b4	-3.654024195	-6.286524195	2.6325			
qmof-f3daf4c	-3.495463333	-7.302119333	3.806656			
qmof-f522cce	-3.118228008	-6.462344008	3.344116			
qmof-1b76fc2	-2.792262837	-6.660186837	3.867924			
qmof-182ba74	-3.604987138	-7.532099138	3.927112			
qmof-7a701d8	-3.136547446	-5.673217446	2.53667			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-1bef540	-3.390805609	-5.900849609	2.510044			
qmof-e0af624	-3.211810352	-7.124173352	3.912363			
qmof-1a3858d	-3.152558373	-7.232653373	4.080095			
qmof-8b03127	-3.782714585	-6.216354585	2.43364	✓		
qmof-fd6d700	-3.679555152	-7.010779152	3.331224			
qmof-7685f3d	-2.802074031	-5.889557031	3.087483			
qmof-7ec2a15	-3.402090259	-6.558365259	3.156275			
qmof-25f9758	-2.474933685	-5.429655685	2.954722			
qmof-c4e84a2	-2.717640244	-4.876737244	2.159097			
qmof-146e551	-2.698260202	-4.799952202	2.101692			
qmof-65f536b	-3.342763583	-6.704626583	3.361863			
qmof-d2b80ff	-2.39116049	-4.86294849	2.471788			
qmof-89a5c57	-2.915239737	-4.935526737	2.020287			
qmof-0f7138b	-2.864910826	-5.629407826	2.764497			
qmof-5fa242c	-2.14620929	-5.33422729	3.188018			
qmof-4fbb0a5	-2.180355577	-5.462600577	3.282245			
qmof-0ec2ee1	-2.48274317	-5.71589717	3.233154			
qmof-e96e55e	-4.25605724	-5.95931724	1.70326			
qmof-e2e748b	-2.993394284	-6.304690284	3.311296			
qmof-7b81e21	-3.707381571	-6.898357571	3.190976			
qmof-edfc49d	-2.859750101	-5.578344101	2.718594			
qmof-2c1dcb9	-3.483520667	-6.141213667	2.657693			
qmof-1e2a4e1	-2.899259565	-5.988264565	3.089005			
qmof-974b2cb	-3.505441245	-7.599252245	4.093811			
qmof-2fde3f7	-3.928641103	-6.940652103	3.012011			
qmof-dca4eee	-3.498928734	-7.132356734	3.633428			
qmof-c9351f5	-3.962160033	-6.430727033	2.468567			
qmof-37d5c1e	-3.006336273	-6.322160273	3.315824			
qmof-4d83581	-3.903180859	-6.432634859	2.529454			
qmof-6977d9d	-2.557163793	-4.739256793	2.182093			
qmof-95efdd8	-2.26271146	-6.15911346	3.896402			
qmof-96bfe65	-2.943868838	-5.120090838	2.176222			
qmof-ef3b26e	-3.07855536	-5.58576036	2.507205			
qmof-5f6120f	-4.176650384	-6.166712384	1.990062			
qmof-6d7fe34	-3.662665756	-6.616878756	2.954213			
qmof-06ab3b1	-2.914015677	-6.271132677	3.357117			
qmof-0180057	-2.764402398	-6.125857398	3.361455			
qmof-72acbfo	-3.180627387	-6.867321387	3.686694			
qmof-e100550	-3.420728903	-5.862406903	2.441678	✓	✓	
qmof-43db536	-2.088951275	-6.265425275	4.176474			
qmof-dc0fa21	-2.849685673	-5.236754673	2.387069			
qmof-d5e2472	-2.252434292	-6.866724292	4.61429			
qmof-82cbfbf	-2.437922716	-5.324795716	2.886873			
qmof-3e65b16	-2.490560144	-6.613948144	4.123388			
qmof-35f76d8	-3.223778229	-5.697526229	2.473748	✓	✓	✓
qmof-0315b97	-3.709619813	-6.835803813	3.126184			
qmof-d04a2a3	-3.731355124	-5.576151124	1.844796			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-58cb01d	-3.752926899	-6.006849899	2.253923	✓		
qmof-10cf41c	-3.546948209	-5.901809209	2.354861	✓	✓	
qmof-d3fd7fc	-3.764293037	-6.217906037	2.453613	✓		
qmof-93c87bd	-2.881411047	-5.182665047	2.301254			
qmof-6bf0ec2	-2.760172164	-5.202567164	2.442395			
qmof-21f2274	-3.739964956	-6.568025956	2.828061			
qmof-0154f42	-2.33226252	-4.72015452	2.387892			
qmof-114133e	-2.953846843	-5.186550843	2.232704			
qmof-c064653	-3.066635508	-7.435617508	4.368982			
qmof-f1c984a	-2.723513998	-6.844794998	4.121281			
qmof-77bd44c	-2.553844933	-6.547553934	3.993709			
qmof-399b130	-4.50959618	-8.11092018	3.601324			
qmof-c53c937	-2.95224152	-6.70759952	3.755358			
qmof-21c3882	-2.809103852	-6.510412852	3.701309			
qmof-dc7e5a3	-3.748519762	-6.559956762	2.811437			
qmof-9651473	-2.030491926	-6.381432926	4.350941			
qmof-3597a65	-2.959267033	-5.752301033	2.793034			
qmof-954c057	-2.933268042	-6.189198042	3.25593			
qmof-c82cbb7	-3.464217299	-6.441179299	2.976962			
qmof-ce0c773	-2.980470242	-5.859028242	2.878558			
qmof-26d536e	-2.74538599	-6.73833899	3.992953			
qmof-3417ac3	-3.040880811	-6.070616811	3.029736			
qmof-79c2418	-3.392804449	-6.081793449	2.688989			
qmof-e99de19	-2.163829398	-6.250570398	4.086741			
qmof-20d0f7c	-2.294092835	-6.557875835	4.263783			
qmof-1a00b4b	-3.848699515	-6.093989515	2.24529			
qmof-fbba869	-3.035352784	-7.352903784	4.317551			
qmof-129e3a9	-2.564237635	-6.988632635	4.424395			
qmof-26d6869	-4.099492331	-7.748834331	3.649342			
qmof-6e89a67	-2.992588773	-7.461497773	4.468909			
qmof-f7de712	-2.412259081	-6.469211081	4.056952			
qmof-b2fb769	-2.909899011	-6.669210011	3.759311			
qmof-2d9f5f9	-3.455103518	-5.667087518	2.211984			
qmof-0a13fbf	-3.317059687	-7.119311688	3.802252			
qmof-ad7adbe	-3.297686262	-6.849974262	3.552288			
qmof-e951f69	-2.851324757	-5.030111757	2.178787			
qmof-3301d94	-2.78158712	-5.17288212	2.391295			
qmof-8cd108f	-3.148008786	-6.403312787	3.255304			
qmof-83e56fe	-2.746709145	-6.748436145	4.001727			
qmof-1105864	-1.691944824	-5.681291824	3.989347			
qmof-458a962	-2.382072677	-5.977829677	3.595757			
qmof-cb3abbe	-2.368628855	-5.667099855	3.298471			
qmof-b46a7a6	-2.186397025	-6.364289025	4.177892			
qmof-0c33be9	-2.780651702	-6.591879702	3.811228			
qmof-b4e6ea2	-2.55903942	-6.45915142	3.900112			
qmof-a9f6b42	-4.269502231	-6.310572231	2.04107			
qmof-536a1f0	-3.728798811	-5.722850811	1.994052	✓		

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-3ada75c	-2.736762741	-6.392765741	3.656003			
qmof-fe916fb	-2.138858704	-6.351132704	4.212274			
qmof-0444ac2	-2.630415517	-5.392316517	2.761901			
qmof-a745d46	-2.972454809	-7.293525809	4.321071			
qmof-602401f	-2.073407704	-4.722655704	2.649248			
qmof-2315a54	-2.737806777	-6.561245777	3.823439			
qmof-828f8b4	-3.396713272	-5.246158272	1.849445			
qmof-2001a62	-3.176739166	-6.873353166	3.696614			
qmof-ccdbd1a	-4.26127169	-7.29158269	3.030311			
qmof-f9dc87c	-2.421196605	-6.300338605	3.879142			
qmof-3988bbf	-3.152973788	-6.368350788	3.215377			
qmof-4f2b4da	-1.868937517	-5.453078517	3.584141			
qmof-d06ef43	-2.050234394	-6.063314394	4.01308			
qmof-3d44993	-2.56423081	-6.39046881	3.826238			
qmof-2aa8eb1	-3.508948621	-5.512810621	2.003862			
qmof-36e6f89	-2.69676621	-6.61111821	3.914352			
qmof-4b71659	-2.654979398	-4.981213398	2.326234			
qmof-92b4b13	-3.121244431	-5.324423431	2.203179			
qmof-e5dde7a	-2.596089423	-6.560338423	3.964249			
qmof-44b1658	-2.323193048	-6.589834048	4.266641			
qmof-5d3ef84	-2.50872004	-6.28760504	3.778885			
qmof-b32e4aa	-4.165678365	-7.722311365	3.556633			
qmof-984892e	-3.772826652	-6.165972652	2.393146	✓		
qmof-60f2715	-2.241393273	-4.967191273	2.725798			
qmof-272c907	-2.407776134	-5.125712134	2.717936			
qmof-5dcb48a	-3.256138156	-5.611876156	2.355738			
qmof-04a6cff	-2.74688415	-5.98356815	3.236684			
qmof-0b22857	-3.244393596	-5.488695596	2.244302			
qmof-a8c7976	-1.82607233	-4.09633133	2.270259			
qmof-93ed13d	-3.685997907	-6.951169907	3.265172			
qmof-2b2a726	-1.791565085	-6.182469085	4.390904			
qmof-c136b83	-2.591106111	-4.687786111	2.09668			
qmof-4577c03	-3.914823044	-6.750512044	2.835689			
qmof-00afe28	-3.259712018	-5.351843018	2.092131			
qmof-a879a21	-3.158342131	-5.336796131	2.178454			
qmof-29c6781	-3.122650161	-5.226371161	2.103721			
qmof-36f1e77	-3.203555328	-5.300933328	2.097378			
qmof-3df82ff	-2.647846689	-5.727628689	3.079782			
qmof-4a2d090	-3.248222982	-6.025158983	2.776936			
qmof-8b9c6cf	-1.621558759	-4.578753759	2.957195			
qmof-55e124e	-2.987149061	-5.797483061	2.810334			
qmof-b808abd	-1.9655434	-5.0229564	3.057413			
qmof-04a422b	-2.652016367	-5.136439367	2.484423			
qmof-2cc3702	-2.288989724	-4.483204724	2.194215			
qmof-8636073	-2.012009245	-6.066835245	4.054826			
qmof-c96d53b	-2.282862598	-5.242468598	2.959606			
qmof-692f848	-3.504084162	-7.511601162	4.007517			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-83e4c15	-3.6515237	-7.6010937	3.94957			
qmof-d35757d	-3.646316821	-7.593563821	3.947247			
qmof-5bd1c51	-3.615045589	-7.556305589	3.94126			
qmof-7563546	-3.136677896	-6.365054896	3.228377			
qmof-e8e772c	-4.020714863	-7.500700863	3.479986			
qmof-cb5f8d9	-3.500263439	-6.322246439	2.821983			
qmof-2657d57	-3.325389758	-7.217530758	3.892141			
qmof-13f5324	-2.802713319	-5.379237319	2.576524			
qmof-02650f9	-3.39408396	-5.75721696	2.363133	✓	✓	✓
qmof-7cb4137	-2.995633661	-5.465846661	2.470213			
qmof-a7de9ff	-3.077830382	-6.309932382	3.232102			
qmof-9ac831b	-2.825988981	-6.929875981	4.103887			
qmof-2d64b34	-3.238570591	-5.816173591	2.577603			
qmof-755604a	-2.788475519	-5.247197519	2.458722			
qmof-fe6f735	-1.774562843	-5.903773843	4.129211			
qmof-2fe9d9b	-3.276031108	-6.707648108	3.431617			
qmof-97fc651	-2.792382082	-5.307098082	2.514716			
qmof-f04954c	-3.562680148	-6.511242148	2.948562			
qmof-5ed2725	-4.119067507	-6.165663507	2.046596			
qmof-b430899	-4.179730173	-6.227698173	2.047968			
qmof-561ba01	-5.036358245	-8.459914245	3.423556			
qmof-943fcb0	-4.048849899	-7.675407899	3.626558			
qmof-ce1173f	-2.838119363	-6.572792363	3.734673			
qmof-8e2d290	-3.371825425	-7.531218425	4.159393			
qmof-6d04fee	-2.940948029	-6.983960029	4.043012			
qmof-49b3901	-3.357463182	-5.821622182	2.464159	✓	✓	✓
qmof-6b45ff6	-2.326559872	-6.346575872	4.020016			
qmof-3a22435	-2.73068825	-6.57099525	3.840307			
qmof-c0a33f9	-2.988195841	-6.761805841	3.77361			
qmof-725dfa2	-2.154640727	-5.710956727	3.556316			
qmof-56e3289	-3.68602679	-7.75750279	4.071476			
qmof-bde105e	-2.925476156	-6.123173156	3.197697			
qmof-2f0e858	-2.812721896	-6.168952896	3.356231			
qmof-5e0ed29	-3.377574625	-5.509711625	2.132137			
qmof-faf4b45	-3.125762823	-6.488686823	3.362924			
qmof-9f661a9	-3.727818135	-6.926255135	3.198437			
qmof-3a8aeef	-3.554726184	-6.778718184	3.223992			
qmof-9e4d3cd	-3.408342361	-7.045340361	3.636998			
qmof-1deaa9a	-2.831322603	-6.475503603	3.644181			
qmof-e6d5869	-3.468619424	-7.145125424	3.676506			
qmof-12fff70	-3.36968491	-6.75385091	3.384166			
qmof-0af7444	-3.863347634	-6.023626634	2.160279			
qmof-c330eaf	-1.617259887	-4.693841887	3.076582			
qmof-ccee605	-2.875956315	-6.991093315	4.115137			
qmof-683ccdc	-3.346946427	-6.856700427	3.509754			
qmof-4c4d6c3	-2.448842463	-5.705712463	3.25687			
qmof-4124b8d	-1.89511323	-6.14340023	4.248287			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-b0bde78	-2.551340638	-6.470113638	3.918773			
qmof-66dc50d	-2.905376428	-5.363277428	2.457901			
qmof-275ec22	-1.241007654	-4.714458654	3.473451			
qmof-1013282	-3.094850439	-6.682259439	3.587409			
qmof-a98810e	-3.296637452	-6.549400452	3.252763			
qmof-98dce4c	-2.995718911	-5.377587911	2.381869			
qmof-1f08cd7	-2.653343306	-5.800516306	3.147173			
qmof-ccf41ca	-3.926791931	-7.760935932	3.834144			
qmof-59aa942	-2.958398149	-5.305524149	2.347126			
qmof-2c16169	-3.00893802	-5.06929602	2.060358			
qmof-94898ae	-2.452701654	-6.273690654	3.820989			
qmof-e534471	-4.591490745	-6.452698745	1.861208			
qmof-1a42fad	-4.601410506	-6.627365506	2.025955			
qmof-363e93c	-2.663791477	-6.273171477	3.60938			
qmof-4b38c0b	-2.614909247	-6.519147247	3.904238			
qmof-d383524	-3.885248823	-6.830546823	2.945298			
qmof-bc2bf53	-3.807460172	-5.867304172	2.059844			
qmof-97f4720	-3.801421239	-5.987828239	2.186407			
qmof-966fade	-4.141154385	-6.084250385	1.943096			
qmof-38eac89	-4.059540269	-5.676557269	1.617017			
qmof-87b3bdd	-4.031173479	-6.281313479	2.25014			
qmof-2cf4df0	-2.748286028	-6.071197028	3.322911			
qmof-082c84f	-4.417483367	-6.244475367	1.826992			
qmof-9883216	-2.443955475	-6.275114475	3.831159			
qmof-07fbe14	-2.652718335	-6.613533335	3.960815			
qmof-68010e6	-2.856369245	-4.780834245	1.924465			
qmof-bbb6f1d	-2.747318731	-6.271921731	3.524603			
qmof-f4e3be2	-1.818024221	-6.013102221	4.195078			
qmof-476a5b8	-2.71534911	-6.61256011	3.897211			
qmof-07c91b5	-3.705068614	-6.835694614	3.130626			
qmof-0c64ba3	-2.326459555	-5.612637555	3.286178			
qmof-08a8079	-2.684344758	-6.777154758	4.09281			
qmof-6581895	-4.111943185	-7.788160185	3.676217			
qmof-c45f4aa	-2.301322515	-6.388537515	4.087215			
qmof-12c7df0	-3.025084321	-5.268611321	2.243527			
qmof-3669068	-2.331383954	-6.483740954	4.152357			
qmof-e03dbd5	-3.172113919	-5.71942392	2.54731			
qmof-9f0b3fe	-2.583108133	-4.834368133	2.25126			
qmof-d8224dc	-2.952362165	-4.971310165	2.018948			
qmof-214ca92	-3.811647684	-6.053793684	2.242146			
qmof-7cb301f	-2.7136841	-6.2471321	3.533448			
qmof-60450dd	-2.567983752	-6.056707752	3.488724			
qmof-d44e9a3	-2.411085722	-4.529955722	2.11887			
qmof-4d203e9	-3.31927696	-5.72353396	2.404257	✓	✓	✓
qmof-44c00af	-3.418022811	-5.616590812	2.198568			
qmof-b70466d	-2.168128371	-4.675149371	2.507021			
qmof-b71cc86	-3.021995527	-5.516562527	2.494567			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-439555b	-3.411650301	-7.420209301	4.008559			
qmof-ad7387b	-4.298347479	-6.183870479	1.885523			
qmof-6fcc83e	-4.083127337	-5.842855337	1.759728			
qmof-d513970	-2.833959969	-6.789036969	3.955077			
qmof-7953340	-3.786707063	-5.518000063	1.731293			
qmof-094542b	-4.128790388	-6.114315388	1.985525			
qmof-c906ab4	-2.463514351	-4.804099352	2.340585			
qmof-41bc44e	-2.877740413	-5.341984413	2.464244			
qmof-e6be400	-2.833163769	-5.022905769	2.189742			
qmof-e7f4b5f	-2.964986448	-5.047380448	2.082394			
qmof-e6bb80c	-2.244634431	-5.935004431	3.69037			
qmof-284c1aa	-2.513149247	-5.126548247	2.613399			
qmof-d105fa0	-2.419168255	-6.572901255	4.153733			
qmof-c775fd7	-1.416746132	-6.436931132	5.020185			
qmof-9940a4e	-2.832864964	-6.398913964	3.566049			
qmof-60df73a	-2.303019215	-5.996218215	3.693199			
qmof-bff6e3a	-3.0988367	-6.4573467	3.35851			
qmof-d10ccb2	-2.478764788	-6.043897788	3.565133			
qmof-ab3cb93	-3.00869223	-6.43519423	3.426502			
qmof-b1020c2	-1.640104912	-5.751962912	4.111858			
qmof-dbbcff4	-3.196201642	-6.108714642	2.912513			
qmof-babba36	-3.500601018	-7.237653018	3.737052			
qmof-b13adc9	-2.536972774	-6.182990774	3.646018			
qmof-a915127	-3.421955367	-6.124017367	2.702062			
qmof-18306a5	-2.572727345	-5.959154345	3.386427			
qmof-bc76ca2	-3.339139715	-6.432111715	3.092972			
qmof-b99f6b2	-3.299578055	-7.007839055	3.708261			
qmof-757860d	-3.429886631	-6.641913631	3.212027			
qmof-fa0c5a7	-2.877720096	-6.072097096	3.194377			
qmof-ad44d4e	-3.016308506	-5.572567506	2.556259			
qmof-3dab219	-3.092985636	-5.180492636	2.087507			
qmof-306fb3e	-3.451265222	-5.862715222	2.41145	✓	✓	
qmof-1de625c	-3.571769764	-5.484522764	1.912753			
qmof-3f9372d	-3.235574124	-5.135625124	1.900051			
qmof-591956d	-3.422778936	-5.400326936	1.977548			
qmof-ea963b6	-3.366576777	-5.850112777	2.483536	✓	✓	✓
qmof-8e4eda8	-2.987103563	-5.343514563	2.356411			
qmof-56f4308	-3.332966479	-5.753864479	2.420898	✓	✓	✓
qmof-8f2f198	-2.885324569	-6.338941569	3.453617			
qmof-c098fd3	-2.656623036	-6.235984036	3.579361			
qmof-00e611b	-3.31618643	-6.05789743	2.741711			
qmof-6005a80	-3.00089141	-5.75149341	2.750602			
qmof-53df3c7	-1.861438757	-6.064624757	4.203186			
qmof-299e646	-2.859563815	-5.791592815	2.932029			
qmof-425232b	-1.264996339	-3.394299339	2.129303			
qmof-657a971	-2.922670901	-5.725773901	2.803103			
qmof-3ca5d72	-3.672973333	-5.757929333	2.084956	✓		

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-0782391	-3.050319148	-5.148625148	2.098306			
qmof-902b24f	-3.207688882	-6.753786882	3.546098			
qmof-d12960f	-2.933921136	-6.582653136	3.648732			
qmof-d390079	-2.786992483	-6.762825483	3.975833			
qmof-0b4817e	-3.209447646	-5.149078646	1.939631			
qmof-e68f2b2	-2.019257674	-6.618766674	4.599509			
qmof-93da51e	-4.020308256	-5.972878256	1.95257			
qmof-0df517f	-3.58861018	-5.71028818	2.121678	✓	✓	
qmof-9df80d1	-3.820752891	-7.482931891	3.662179			
qmof-098256e	-2.527519005	-5.499925005	2.972406			
qmof-90df4ad	-2.056122623	-5.297615623	3.241493			
qmof-fe66204	-2.081166187	-5.065236187	2.98407			
qmof-3e96a80	-3.639062619	-6.173149619	2.534087			
qmof-172319f	-3.142822414	-5.462788414	2.319966			
qmof-190cb3e	-2.842552055	-5.455192055	2.61264			
qmof-9ea13da	-2.815476016	-5.435464016	2.619988			
qmof-7bc9775	-3.216987342	-7.003700342	3.786713			
qmof-13463bb	-1.692047158	-5.533466158	3.841419			
qmof-b33b31e	-2.99191112	-5.52479612	2.532885			
qmof-b517439	-3.247244264	-6.191886264	2.944642			
qmof-d270b21	-3.386182345	-6.160286345	2.774104			
qmof-a1d95f7	-3.410527545	-5.319079545	1.908552			
qmof-0e0cf73	-3.583942527	-6.996366527	3.412424			
qmof-5bcace3	-3.312818731	-7.385754731	4.072936			
qmof-3bda7fc	-3.199021512	-6.598745512	3.399724			
qmof-4125488	-2.970107686	-5.088879686	2.118772			
qmof-5dfc500	-0.595081699	-4.4261637	3.831082			
qmof-439bd40	-2.336211728	-5.597278728	3.261067			
qmof-99ecd48	-3.413935342	-6.436992342	3.023057			
qmof-acc11bc	-3.375085838	-6.375323838	3.000238			
qmof-26888fa	-2.720968172	-4.887558172	2.16659			
qmof-d73b859	-3.097844499	-7.127774499	4.02993			
qmof-0fbfb10	-2.806967078	-5.584385078	2.777418			
qmof-ea27d90	-2.877129614	-5.711361614	2.834232			
qmof-bd3dde7	-2.949257586	-6.951235586	4.001978			
qmof-2d80bfd	-1.633136737	-4.888485737	3.255349			
qmof-69add22	-3.096544119	-5.476392119	2.379848			
qmof-6a17ede	-4.196049141	-6.906268141	2.710219			
qmof-9c5aaea	-2.915274304	-6.478837304	3.563563			
qmof-c389047	-2.678991183	-6.778994183	4.100003			
qmof-c8df599	-2.801303818	-5.652830818	2.851527			
qmof-caea536	-4.322321042	-6.258871042	1.93655			
qmof-c0331cb	-3.132882935	-5.579770935	2.446888			
qmof-211265f	-2.294670318	-4.780885318	2.486215			
qmof-e0dc4ed	-2.97608078	-5.49168178	2.515601			
qmof-b0214d8	-3.385194505	-6.432266505	3.047072			
qmof-4c18ced	-2.159646199	-5.991370199	3.831724			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-12edc8c	-2.82902379	-6.47680379	3.64778			
qmof-92f0814	-2.379702292	-5.507839292	3.128137			
qmof-c3d8aec	-3.515054094	-7.064161094	3.549107			
qmof-e5ef618	-2.708182533	-5.592020533	2.883838			
qmof-44c1049	-2.797660758	-5.196303758	2.398643			
qmof-5d9fab0	-2.236528067	-5.715985067	3.479457			
qmof-9fbdc0b	-2.859985143	-6.540497143	3.680512			
qmof-e5e12e2	-2.751625229	-6.242108229	3.490483			
qmof-2c408e6	-2.839543702	-5.363779702	2.524236			
qmof-0f178f1	-1.865379063	-4.919521063	3.054142			
qmof-f0dfa44	-2.107125686	-4.904047686	2.796922			
qmof-59b517c	-2.406160079	-6.629101079	4.222941			
qmof-ef42d2a	-2.839726319	-5.171428319	2.331702			
qmof-c0bdee5	-3.621783077	-5.624786077	2.003003			
qmof-0e4bbcb	-3.276843311	-6.166381311	2.889538			
qmof-17b62c4	-2.956136876	-6.923141876	3.967005			
qmof-70f4cf7	-3.797253691	-6.252861691	2.455608			
qmof-a0e80c5	-5.433586437	-8.503804437	3.070218			
qmof-4ac7df5	-2.36400421	-6.19488521	3.830881			
qmof-d429569	-4.373482256	-7.823681256	3.450199			
qmof-f9e6ec3	-2.030252992	-5.237195992	3.206943			
qmof-d83a3a6	-3.137349139	-6.483560139	3.346211			
qmof-c988bec	-3.044310331	-5.966587331	2.922277			
qmof-1b44fef	-2.313322909	-5.550733909	3.237411			
qmof-1580a8b	-3.313579452	-6.447970452	3.134391			
qmof-2e02fed	-2.892159331	-6.309550331	3.417391			
qmof-c9f20d8	-3.240000262	-5.570721262	2.330721			
qmof-2593f7a	-2.099493899	-6.391715899	4.292222			
qmof-9a7a515	-2.346616347	-4.607376347	2.26076			
qmof-ad5034e	-3.494881742	-5.454344742	1.959463			
qmof-1a49402	-3.803591324	-7.219236324	3.415645			
qmof-6777158	-2.784679157	-6.643959157	3.85928			
qmof-877d368	-3.559820755	-5.584941755	2.025121			
qmof-a89b009	-1.512735402	-4.485122402	2.972387			
qmof-cd31982	-3.905924166	-6.854759166	2.948835			
qmof-b0fd440	-3.402458178	-6.267049178	2.864591			
qmof-1e427c5	-2.528184333	-6.343980333	3.815796			
qmof-b5d466b	-3.117396327	-6.717177327	3.599781			
qmof-5c8908e	-3.294463243	-5.922552243	2.628089			
qmof-c0a61f9	-2.912370635	-5.679639635	2.767269			
qmof-16dd495	-2.879458048	-6.738271048	3.858813			
qmof-57e2359	-2.393979685	-4.545357685	2.151378			
qmof-c49d30b	-1.227532795	-5.336592795	4.10906			
qmof-2389400	-1.961282017	-5.667157017	3.705875			
qmof-a7ea515	-3.465475896	-6.117236896	2.651761			
qmof-067b298	-3.19614555	-5.63315755	2.437012			
qmof-92f3405	-1.930471223	-5.346804223	3.416333			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-8a2fa8a	-3.257122797	-5.884112797	2.62699			
qmof-80852fd	-2.231648021	-6.119372021	3.887724			
qmof-41301bd	-2.049949252	-6.131244252	4.081295			
qmof-e029d32	-3.424470714	-6.850678714	3.426208			
qmof-98ad58c	-3.344150041	-7.598567041	4.254417			
qmof-d6e31ae	-2.293234719	-4.990978719	2.697744			
qmof-8ccd305	-1.980981112	-4.495124112	2.514143			
qmof-dce5b26	-2.850713169	-5.346429169	2.495716			
qmof-6db4857	-2.472751578	-6.003991578	3.53124			
qmof-88b90c9	-2.011375371	-5.242454371	3.231079			
qmof-6919937	-2.936410704	-6.707841704	3.771431			
qmof-4a54aa8	-3.723444586	-6.595967586	2.872523			
qmof-0344ac0	-2.645074539	-6.528352539	3.883278			
qmof-34239b6	-2.154874678	-6.243443678	4.088569			
qmof-f0e967a	-1.13930451	-5.76937451	4.63007			
qmof-6346309	-2.966138005	-7.077976005	4.111838			
qmof-0906587	-4.664137315	-8.265907315	3.60177			
qmof-35f10de	-2.775515919	-6.188410919	3.412895			
qmof-37e26c7	-4.149383552	-5.544044552	1.394661			
qmof-925aafd	-2.926606299	-6.777640299	3.851034			
qmof-20f3edb	-3.077180232	-6.271530232	3.19435			
qmof-3c5676c	-2.89776312	-6.56237212	3.664609			
qmof-0aaa20a	-2.838001526	-5.915506526	3.077505			
qmof-b11bf9e	-3.129500724	-6.636126724	3.506626			
qmof-c51a724	-3.032359602	-6.458701602	3.426342			
qmof-18b151e	-3.563843167	-7.074221167	3.510378			
qmof-edbe499	-2.901177689	-5.812179689	2.911002			
qmof-437fb3b	-3.435021722	-6.794263722	3.359242			
qmof-004e466	-3.0714245	-6.3452845	3.27386			
qmof-9060c8b	-2.588715498	-6.085281498	3.496566			
qmof-dd09d8f	-3.363071833	-6.138252833	2.775181			
qmof-b537f4f	-3.474866208	-6.075909208	2.601043			
qmof-b544b11	-3.677962984	-7.096911984	3.418949			
qmof-303c74f	-3.542467282	-5.770071282	2.227604	✓	✓	
qmof-b3f1619	-2.554767394	-6.247415394	3.692648			
qmof-648c41f	-2.63566203	-6.98154003	4.345878			
qmof-88c6ebd	-3.618802992	-7.259700992	3.640898			
qmof-003f026	-4.603689163	-7.043713163	2.440024			
qmof-09eb351	-2.636855284	-5.750775284	3.11392			
qmof-f1b0a1e	-4.198231174	-6.587118174	2.388887			
qmof-8ac4d87	-4.181875598	-6.602243598	2.420368			
qmof-c158d1f	-4.207860786	-6.620028786	2.412168			
qmof-204bfd2	-3.482946187	-7.144139187	3.661193			
qmof-fc17802	-3.019618856	-5.852576856	2.832958			
qmof-b127925	-2.642308949	-6.655588949	4.01328			
qmof-12e958e	-2.557575673	-6.157477673	3.599902			
qmof-a52b53c	-2.209249813	-5.379801813	3.170552			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-639e83a	-2.14644904	-6.25084404	4.104395			
qmof-b156e7f	-2.421782459	-5.351758459	2.929976			
qmof-dc694ac	-3.62042833	-6.55670533	2.936277			
qmof-9a204c1	-2.714674461	-6.584000461	3.869326			
qmof-5533c80	-2.704043994	-6.437898994	3.733855			
qmof-b8000f1	-3.093303576	-7.170054576	4.076751			
qmof-85fbc0d	-1.477012772	-5.150547772	3.673535			
qmof-0b7af5b	-2.464071954	-6.053568954	3.589497			
qmof-469075b	-2.553979323	-6.478795323	3.924816			
qmof-1e1bf28	-3.130311846	-6.218611846	3.0883			
qmof-4e113a2	-3.021760654	-7.186975654	4.165215			
qmof-13acee7	-2.751628868	-5.455106868	2.703478			
qmof-792ff35	-2.843439979	-6.818873979	3.975434			
qmof-dbc27ec	-2.946643114	-5.847545114	2.900902			
qmof-47dde23	-3.693086988	-6.525237988	2.832151			
qmof-7b5e892	-1.648467983	-5.626700983	3.978233			
qmof-a51b2a6	-3.749950282	-5.764044282	2.014094	✓		
qmof-a09abf4	-1.930466255	-4.172901255	2.242435			
qmof-39d4547	-3.058215404	-7.049885404	3.99167			
qmof-b4bad2f	-2.584772664	-6.385081664	3.800309			
qmof-458f21b	-3.530167361	-5.839258361	2.309091	✓	✓	
qmof-460d167	-2.65556489	-4.47794389	1.822379			
qmof-d5697d2	-2.728058973	-6.443872973	3.715814			
qmof-7c7b193	-2.054023442	-6.470357442	4.416334			
qmof-fd9adfa	-2.685953441	-5.596099441	2.910146			
qmof-5cd94b8	-2.850514275	-6.758618275	3.908104			
qmof-a6f4cc1	-3.052419451	-5.600084451	2.547665			
qmof-47d81d6	-3.177094393	-7.359135393	4.182041			
qmof-687e4d6	-2.783930902	-6.205854902	3.421924			
qmof-d8bbac8	-2.306566973	-5.899515973	3.592949			
qmof-bf50ae7	-2.598488679	-5.224755679	2.626267			
qmof-e2276ee	-3.334568957	-5.487613957	2.153045			
qmof-effdd4d	-2.377422481	-6.338503481	3.961081			
qmof-d962920	-2.848573427	-6.368099427	3.519526			
qmof-7e13f90	-3.498848517	-5.942190517	2.443342	✓	✓	
qmof-e89cb56	-2.692696377	-5.281200377	2.588504			
qmof-cd42f10	-2.433602159	-6.558297159	4.124695			
qmof-694381f	-2.480596654	-6.188580654	3.707984			
qmof-3f0a2ed	-3.171618167	-5.528695167	2.357077			
qmof-053334d	-2.918923891	-6.272602891	3.353679			
qmof-743e1bf	-2.855936045	-6.854782045	3.998846			
qmof-405a87b	-3.436483946	-7.001477946	3.564994			
qmof-897ea77	-3.388496256	-6.539575256	3.151079			
qmof-d6798a9	-2.900411054	-5.647642054	2.747231			
qmof-ec55375	-2.472951506	-6.287926506	3.814975			
qmof-16738f7	-2.579347683	-5.115440683	2.536093			
qmof-de0737b	-3.09376403	-5.49022403	2.39646			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-9174c13	-3.503124965	-5.949034965	2.44591	✓	✓	
qmof-145af0e	-1.97575046	-6.18251146	4.206761			
qmof-9188690	-3.237149298	-5.298286298	2.061137			
qmof-2ade4ad	-3.153094582	-7.350446582	4.197352			
qmof-4e43b18	-3.596166062	-6.119726062	2.52356			
qmof-9f315fd	-2.758936823	-4.829245823	2.070309			
qmof-593a48e	-2.389890834	-5.971447834	3.581557			
qmof-d481578	-5.01246144	-7.15127444	2.138813			
qmof-053dc27	-3.884954507	-7.169891507	3.284937			
qmof-9fe4370	-3.235626398	-6.855304398	3.619678			
qmof-e80fd66	-3.411612343	-6.801110343	3.389498			
qmof-2d93e62	-4.421981935	-6.838969935	2.416988			
qmof-9a8fdd8	-2.749086328	-6.429730328	3.680644			
qmof-9044ea9	-2.84469524	-6.82762124	3.982926			
qmof-9fa0d98	-3.356703657	-5.816337657	2.459634	✓	✓	✓
qmof-4d684e3	-3.435038995	-5.684234995	2.249196	✓	✓	
qmof-13ec2a4	-3.079553316	-5.090633316	2.01108			
qmof-2a8957f	-2.15701657	-5.59786957	3.440853			
qmof-3336366	-3.225588489	-5.975514489	2.749926			
qmof-e7c726e	-3.101014757	-6.283023757	3.182009			
qmof-375c7bc	-3.004500838	-6.420609838	3.416109			
qmof-8342c5f	-3.754805033	-7.883792033	4.128987			
qmof-6c38eb4	-3.620655513	-6.483048513	2.862393			
qmof-421f50d	-3.24478565	-7.72310465	4.478319			
qmof-45aee87	-2.21177105	-6.36386505	4.152094			
qmof-a42d702	-3.04780317	-5.36436217	2.316559			
qmof-a36c542	-2.685708176	-5.130850176	2.445142			
qmof-182d6dc	-2.802352497	-6.598311497	3.795959			
qmof-f49b443	-3.880389115	-7.720443115	3.840054			
qmof-c530710	-3.575844386	-5.976864386	2.40102	✓	✓	
qmof-9b79393	-2.871839003	-6.750838003	3.878999			
qmof-8e732a8	-1.767901558	-4.441586558	2.673685			
qmof-1eea8fc	-4.068070317	-6.509233317	2.441163			
qmof-981431f	-3.431424744	-6.629473744	3.198049			
qmof-030e486	-3.705022202	-6.661330202	2.956308			
qmof-12c6f7b	-2.564507458	-5.732857458	3.16835			
qmof-98f643f	-3.175222174	-4.839945174	1.664723			
qmof-a653a76	-2.187537626	-6.115909626	3.928372			
qmof-78f6bfc	-3.96748466	-6.67055666	2.703072			
qmof-1c721d8	-3.948964769	-6.675454769	2.72649			
qmof-ccf3de7	-3.199610653	-6.776709653	3.577099			
qmof-ff432b6	-2.593937054	-6.213580054	3.619643			
qmof-10ddadb	-3.048364224	-7.067428224	4.019064			
qmof-6e4326e	-1.722427368	-6.395761368	4.673334			
qmof-7a361fd	-4.45042155	-7.10415355	2.653732			
qmof-8cdca87	-3.775616517	-6.687951517	2.912335			
qmof-5edf8d7	-2.530425119	-6.73116612	4.200741			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-edd4ef0	-2.570717364	-5.597223364	3.026506			
qmof-f72ed6d	-3.296930885	-6.807410885	3.51048			
qmof-684e6eb	-1.740563055	-5.300318055	3.559755			
qmof-cad1202	-1.012303103	-2.694691103	1.682388			
qmof-a123871	-3.34141351	-6.35793251	3.016519			
qmof-70f59fa	-3.731078524	-5.853111524	2.122033	✓		
qmof-4774c35	-3.032415786	-5.558078786	2.525663			
qmof-1a922d4	-2.617369676	-5.040286676	2.422917			
qmof-9ff30cc	-3.298234249	-6.081293249	2.783059			
qmof-831f088	-3.146216875	-7.178289875	4.032073			
qmof-08b67ba	-2.170746008	-5.843601008	3.672855			
qmof-6247dea	-3.00015056	-7.21704756	4.216897			
qmof-d03c776	-2.823705897	-5.165542897	2.341837			
qmof-65f6051	-2.129787915	-4.870870915	2.741083			
qmof-d68a206	-4.288716908	-6.485285908	2.196569			
qmof-67dd780	-2.000497701	-6.596921701	4.596424			
qmof-11a9c18	-2.960144263	-6.681907263	3.721763			
qmof-00744ff	-3.787484096	-6.254153096	2.466669	✓		
qmof-f2fe5ba	-3.322317615	-7.055397615	3.73308			
qmof-453d314	-3.633522403	-6.191726403	2.558204			
qmof-b7f954d	-2.28231169	-5.61687469	3.334563			
qmof-b87071b	-3.489870038	-6.298367038	2.808497			
qmof-728c062	-3.882114293	-5.943099293	2.060985			
qmof-80be546	-4.577884281	-7.142736281	2.564852			
qmof-824f9fd	-3.080124115	-6.418612115	3.338488			
qmof-a9f2188	-3.441285582	-6.806970582	3.365685			
qmof-514abfb	-3.108783114	-6.943687114	3.834904			
qmof-8bbd7b4	-2.307119003	-4.338088003	2.030969			
qmof-4c97440	-3.573327134	-5.619210134	2.045883			
qmof-e2d2c46	-2.722819711	-5.337073711	2.614254			
qmof-545c247	-3.70799563	-6.02244563	2.31445	✓		
qmof-8366080	-3.097723401	-5.730572401	2.632849			
qmof-3f10a21	-2.225393815	-6.378914815	4.153521			
qmof-7d6715f	-2.027720041	-6.248393041	4.220673			
qmof-b023388	-2.286142758	-6.475978758	4.189836			
qmof-b77db05	-3.057041551	-7.101287551	4.044246			
qmof-9d8bf1c	-2.993525952	-6.101482952	3.107957			
qmof-25af73a	-2.72219188	-5.75793688	3.035745			
qmof-0e72b85	-4.170675377	-6.898718377	2.728043			
qmof-1665525	-3.034369386	-5.906634386	2.872265			
qmof-c8f72fc	-2.867602845	-6.173621845	3.306019			
qmof-5ce36bf	-3.082558578	-7.212115578	4.129557			
qmof-9d07fdc	-2.612635741	-5.020923741	2.408288			
qmof-718ab88	-2.013547262	-5.050762262	3.037215			
qmof-e4f98a0	-3.114854475	-5.186058475	2.071204			
qmof-9433b10	-3.975077495	-5.584406495	1.609329			
qmof-4b3dce4	-3.082278089	-6.725212089	3.642934			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-8ccaa8e	-3.837247835	-6.366129835	2.528882			
qmof-fd023ea	-3.068805551	-6.838527551	3.769722			
qmof-03cca0a	-3.398376378	-6.278248378	2.879872			
qmof-7076722	-2.271702138	-5.989789138	3.718087			
qmof-e88ad2b	-3.397066193	-6.070156193	2.67309			
qmof-9653578	-2.85163658	-5.26837458	2.416738			
qmof-ab32015	-3.522333069	-5.570288069	2.047955			
qmof-7dbddd2	-3.942889441	-7.402157441	3.459268			
qmof-545a299	-4.047937279	-7.673050279	3.625113			
qmof-fd388d5	-3.784298011	-7.448817011	3.664519			
qmof-3b9b0b0	-4.446195176	-8.042978176	3.596783			
qmof-9513924	-4.280505958	-7.915692958	3.635187			
qmof-ddefcd4	-3.481243605	-7.029964605	3.548721			
qmof-2f9f102	-4.020142757	-7.663770757	3.643628			
qmof-a9114c3	-3.45694835	-6.96311235	3.506164			
qmof-c98e6d4	-4.27238121	-7.87227921	3.599898			
qmof-00a989b	-3.484616757	-6.966588757	3.481972			
qmof-e273077	-4.017296803	-7.667302803	3.650006			
qmof-0f5fd80	-3.477442699	-6.9978567	3.520414			
qmof-7193001	-2.871573703	-5.302549703	2.430976			
qmof-3a8ae72	-2.585511666	-5.320708666	2.735197			
qmof-a5c1558	-2.336292216	-6.317738216	3.981446			
qmof-00e18cb	-2.489978686	-6.503784686	4.013806			
qmof-a62b5e5	-3.239858625	-6.318178625	3.07832			
qmof-8e256bb	-3.020740022	-7.007540022	3.9868			
qmof-4d8929f	-3.373840473	-5.578118473	2.204278			
qmof-6903e0b	-3.042800756	-6.613514756	3.570714			
qmof-00f4cb5	-3.259930648	-7.219308648	3.959378			
qmof-7dd9b74	-2.200382156	-5.789304156	3.588922			
qmof-5319a12	-2.105080575	-4.639854575	2.534774			
qmof-5982646	-2.392581363	-4.946191363	2.55361			
qmof-9ae3430	-2.34304134	-4.93786734	2.594826			
qmof-b23591b	-2.315715418	-4.579113418	2.263398			
qmof-11f5df1	-2.584822412	-5.984402412	3.39958			
qmof-1a45ce8	-3.401027846	-6.370408846	2.969381			
qmof-81af911	-3.221825546	-6.903972546	3.682147			
qmof-ae1a15f	-2.57018598	-6.44847998	3.878294			
qmof-2c7948e	-2.858622109	-6.320897109	3.462275			
qmof-3d17539	-3.014872662	-5.367330662	2.352458			
qmof-63d089a	-2.315166548	-5.806330548	3.491164			
qmof-6f8a430	-2.285909157	-6.290476157	4.004567			
qmof-855d1ed	-2.910192366	-6.681418366	3.771226			
qmof-cb3b518	-2.573579187	-6.163238187	3.589659			
qmof-6c6014c	-2.722219414	-5.777845414	3.055626			
qmof-9e7a580	-3.593102223	-6.483692223	2.89059			
qmof-d53e130	-2.65941013	-5.68020913	3.020799			
qmof-73b7fe4	-3.497508628	-7.260231628	3.762723			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-88ffdd8	-3.125516702	-7.081449702	3.955933			
qmof-7c7b7c4	-3.001721638	-6.315149638	3.313428			
qmof-042db04	-2.852820261	-5.212960261	2.36014			
qmof-2b351d2	-3.092329353	-5.222188353	2.129859			
qmof-43a9124	-4.116633081	-6.900131081	2.783498			
qmof-6204da9	-4.192161015	-6.936663015	2.744502			
qmof-a42e6fd	-3.019553329	-6.879918329	3.860365			
qmof-358d837	-3.124361127	-7.029102127	3.904741			
qmof-4cbd9c7	-2.926710795	-5.411555795	2.484845			
qmof-28770b1	-2.143617526	-6.355244526	4.211627			
qmof-da4d665	-2.692816783	-6.603487783	3.910671			
qmof-3816edb	-3.990710849	-8.288672849	4.297962			
qmof-7322852	-3.213572848	-6.115196848	2.901624			
qmof-eb98c8b	-1.386854009	-4.778083009	3.391229			
qmof-b5f87de	-2.718715583	-5.063534583	2.344819			
qmof-ab54701	-2.516442947	-6.976035947	4.459593			
qmof-ca6a000	-3.641644656	-7.238722656	3.597078			
qmof-cb3e9e8	-3.63036647	-7.04477147	3.414405			
qmof-3a1b292	-2.26531202	-5.69082402	3.425512			
qmof-18442f6	-2.964795433	-7.107579433	4.142784			
qmof-d6d8373	-3.569957137	-5.746673137	2.176716	✓	✓	
qmof-0454c23	-3.263707752	-5.694420752	2.430713	✓	✓	✓
qmof-7dfd503	-3.490613483	-5.499893483	2.00928			
qmof-268a4cf	-2.540990088	-5.636327088	3.095337			
qmof-d028335	-2.733384779	-6.508366779	3.774982			
qmof-165659f	-2.061068648	-6.040341648	3.979273			
qmof-28aae3b	-2.448502078	-6.437180078	3.988678			
qmof-66698de	-2.943909665	-5.446661665	2.502752			
qmof-7f0e6bf	-2.811628999	-6.190323999	3.378695			
qmof-0091475	-3.659419622	-5.747818622	2.088399	✓		
qmof-89f6056	-1.681030708	-5.348993708	3.667963			
qmof-a0b0c6b	-4.673154564	-8.670758564	3.997604			
qmof-8e16ab1	-2.796424338	-6.524640338	3.728216			
qmof-8dcabcf	-1.099070199	-5.524896199	4.425826			
qmof-5075011	-4.051778094	-7.175604094	3.123826			
qmof-00f576b	-2.634818037	-6.501990037	3.867172			
qmof-1fe9d39	-3.618048351	-5.615384351	1.997336			
qmof-a3a09fc	-3.284201867	-7.551314867	4.267113			
qmof-add8947	-3.897359561	-6.014999561	2.11764			
qmof-bcdc0ff	-3.811004859	-5.933495859	2.122491			
qmof-0267c10	-3.805098621	-7.280041621	3.474943			
qmof-534fef5	-4.133861385	-5.686487385	1.552626			
qmof-611de0b	-2.96538946	-6.67995446	3.714565			
qmof-20e559b	-4.290701918	-6.696212918	2.405511			
qmof-9f6fc79	-4.691188308	-7.212627308	2.521439			
qmof-ca683eb	-3.338756881	-6.471267881	3.132511			
qmof-6d0ce1c	-3.038633018	-7.156717018	4.118084			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-26d0da3	-2.628447953	-6.092386953	3.463939			
qmof-006d43a	-2.96341153	-5.646549531	2.683138			
qmof-633a43e	-2.529076566	-5.581735566	3.052659			
qmof-9cfc8a3	-4.091221495	-7.676054495	3.584833			
qmof-5038232	-2.474546419	-6.106847419	3.632301			
qmof-86b73f0	-3.376140889	-7.656960889	4.28082			
qmof-10c7c3c	-3.428646023	-6.713862023	3.285216			
qmof-d84f27e	-3.760578396	-6.721743396	2.961165			
qmof-5be3f38	-3.32469994	-7.27490594	3.950206			
qmof-9dd2a8a	-1.213890862	-5.173052862	3.959162			
qmof-50a4b12	-2.388914918	-5.120110918	2.731196			
qmof-a326ecc	-2.34562141	-5.12699741	2.781376			
qmof-1f153d6	-3.145628646	-5.591462646	2.445834			
qmof-222a152	-3.024206434	-5.431912434	2.407706			
qmof-ef126da	-3.387553317	-5.594369317	2.206816			
qmof-c398fa7	-3.098662553	-5.446269553	2.347607			
qmof-0091bbc	-2.648027209	-4.94843021	2.300403			
qmof-23be8ef	-3.040908678	-5.314572678	2.273664			
qmof-21a886a	-3.486722181	-5.460580181	1.973858			
qmof-b9094ed	-3.5362459	-6.5144949	2.978249			
qmof-3643545	-3.220183601	-6.953816601	3.733633			
qmof-d856602	-3.451038607	-6.519330607	3.068292			
qmof-204eab0	-3.58714766	-6.53393266	2.946785			
qmof-564af28	-3.372509861	-5.214732861	1.842223			
qmof-15f7608	-3.401078547	-5.195238547	1.79416			
qmof-747ed4e	-3.514462248	-5.605512248	2.09105			
qmof-82a687d	-3.511447743	-5.629625743	2.118178			
qmof-2aecb3c	-3.770755194	-6.353516194	2.582761			
qmof-acb9b4e	-2.446230497	-5.024585497	2.578355			
qmof-2888e3d	-3.404757395	-7.515779395	4.111022			
qmof-435674b	-2.389249336	-6.475435336	4.086186			
qmof-f130ab1	-1.487597738	-4.963432738	3.475835			
qmof-fc193c1	-1.561559592	-5.055779592	3.49422			
qmof-7c7fd1a	-2.448637063	-6.230307063	3.78167			
qmof-12d18bf	-5.119675371	-5.194567371	0.074892			
qmof-f57add2	-2.871209269	-6.500462269	3.629253			
qmof-f4a5f09	-3.350199145	-7.228186145	3.877987			
qmof-5b4423d	-3.09078357	-6.60528357	3.5145			
qmof-cc0269e	-3.698773335	-6.257349335	2.558576			
qmof-8c2860b	-3.373699967	-6.835297967	3.461598			
qmof-27e3cca	-2.731544294	-5.625090294	2.893546			
qmof-d8703ab	-2.280957477	-5.619604477	3.338647			
qmof-277fc99	-3.311175379	-5.345183379	2.034008			
qmof-28e1e79	-2.513595213	-6.490240213	3.976645			
qmof-3cfc4c8	-2.42048096	-5.17609496	2.755614			
qmof-8be7b17	-2.59404546	-6.54116046	3.947115			
qmof-5f3f601	-0.51669152	-2.47012652	1.953435			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-39c37e1	-3.832250686	-6.455622686	2.623372	✓		
qmof-cef46c3	-3.2496281	-6.1787091	2.929081			
qmof-826d4fe	-2.652127031	-6.142436031	3.490309			
qmof-1658787	-2.212941007	-4.757514007	2.544573			
qmof-98f79b2	-3.783130811	-5.892228811	2.109098			
qmof-d690c9a	-4.028552274	-6.198789274	2.170237			
qmof-7dd3a77	-4.017710568	-6.083586568	2.065876			
qmof-02c0106	-3.007222944	-7.015975944	4.008753			
qmof-417cefc	-2.283832563	-6.291040563	4.007208			
qmof-79ff2bd	-3.430545195	-6.641135195	3.21059			
qmof-c312b02	-3.699287967	-6.573490967	2.874203			
qmof-19e8f60	-3.065972158	-6.562338158	3.496366			
qmof-aa0100a	-1.526759602	-4.792118602	3.265359			
qmof-a2a082e	-1.784461158	-5.204887158	3.420426			
qmof-7acc00d	-2.716071427	-6.487954427	3.771883			
qmof-2fa85e9	-2.360511681	-6.352213681	3.991702			
qmof-f771839	-2.537810572	-6.589959572	4.052149			
qmof-6f5eeb5	-3.118164647	-5.963096647	2.844932			
qmof-06b3283	-2.9178014	-6.6263274	3.708526			
qmof-1278662	-1.207994592	-5.204099592	3.996105			
qmof-c3de041	-2.179177185	-6.468826185	4.289649			
qmof-46fd06d	-3.112193559	-6.591690559	3.479497			
qmof-8cdd2eb	-4.630376063	-6.880651063	2.250275			
qmof-cdab0e2	-3.959788706	-6.231220706	2.271432			
qmof-eda34e0	-3.095286543	-5.414533543	2.319247			
qmof-5c23399	-3.000813132	-7.007697132	4.006884			
qmof-32a3837	-3.494090633	-6.143437633	2.649347	✓		
qmof-59fd38f	-2.683290109	-6.631173109	3.947883			
qmof-976a1e2	-3.661267201	-5.746927201	2.08566			
qmof-163ccaa	-4.324807864	-6.788606864	2.463799			
qmof-391d6b2	-3.898339306	-6.202168306	2.303829			
qmof-de01c79	-4.188988299	-6.612462299	2.423474			
qmof-3254029	-2.839419435	-6.674748435	3.835329			
qmof-177ecfa	-3.3911908	-5.9393398	2.548149			
qmof-a76ae33	-3.458983755	-6.272572755	2.813589			
qmof-eab8e84	-4.341226143	-6.799482143	2.458256			
qmof-db46c4e	-3.233796605	-7.575097605	4.341301			
qmof-850f45a	-2.438195205	-6.334314205	3.896119			
qmof-6f77b06	-2.790593054	-5.848467054	3.057874			
qmof-844af13	-2.564989793	-5.807173793	3.242184			
qmof-8746f65	-3.239040307	-6.642998307	3.403958			
qmof-9da8e10	-4.071553401	-6.317356401	2.245803			
qmof-ab01344	-2.409356638	-6.506258638	4.096902			
qmof-7abf8f7	-2.376888508	-6.485930508	4.109042			
qmof-fd6b778	-2.3992126	-6.4864886	4.087276			
qmof-73ef0e4	-2.272814078	-6.495501078	4.222687			
qmof-5bdd458	-2.223555783	-5.811066783	3.587511			

Continued on next page

Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-5f3eef5	-2.740683405	-6.072780405	3.332097			
qmof-a0774e6	-2.325215848	-5.154574848	2.829359			
qmof-9852a98	-2.633317776	-5.317120776	2.683803			
qmof-c7fbe0d	-2.964515886	-6.437026886	3.472511			
qmof-799305a	-2.067234305	-5.498567305	3.431333			
qmof-c00d6a1	-2.832692955	-5.805440955	2.972748			
qmof-d45c96f	-2.960803367	-4.985343367	2.02454			
qmof-d8b5d6f	-3.560478503	-6.115178503	2.5547			
qmof-3847280	-2.63023092	-4.83056692	2.200336			
qmof-57bb27b	-2.462954095	-6.115600095	3.652646			
qmof-cdc2b7e	-2.942568554	-5.801761554	2.859193			
qmof-201ddfa	-3.07566507	-6.89981807	3.824153			
qmof-bb9d22a	-2.97770893	-7.18169593	4.203987			
qmof-2959e3b	-3.681230503	-8.147426503	4.466196			
qmof-caff655	-3.540193015	-5.731544015	2.191351	✓	✓	
qmof-dbfb0b69	-2.98893515	-5.58745315	2.598518			
qmof-1794723	-2.286505495	-4.495519495	2.209014			
qmof-b8f1b55	-2.202103011	-4.724149011	2.522046			
qmof-dfed9ce	-3.106555814	-5.373081814	2.266526			
qmof-3f2cc61	-1.85801642	-4.72992642	2.87191			
qmof-cb7fcfc	-2.767850819	-5.983876819	3.216026			
qmof-3465f36	-1.924474471	-4.976319471	3.051845			
qmof-170efc8	-3.194620349	-5.712350349	2.51773			
qmof-7c3b12f	-2.853336258	-5.489789258	2.636453			
qmof-c4a4198	-4.076956088	-6.187076088	2.11012			
qmof-14e4ce3	-2.614566194	-6.574462194	3.959896			
qmof-ec1edf9	-3.294334827	-5.971098827	2.676764			
qmof-2030d07	-3.161323438	-5.756608438	2.595285			
qmof-0507e96	-3.220826802	-7.107526802	3.8867			
qmof-5486f8c	-3.182342594	-7.201242594	4.0189			
qmof-859646d	-3.025888285	-7.235565285	4.209677			
qmof-bd72da2	-2.927867317	-5.405127317	2.47726			
qmof-2c4a8be	-2.68318714	-6.14113714	3.45795			
qmof-cc4910d	-2.384030446	-5.346624446	2.962594			
qmof-bb2839a	-3.034513065	-5.696021065	2.661508			
qmof-b7815da	-2.197676181	-6.544029181	4.346353			
qmof-63cb6eb	-1.591470934	-5.721265934	4.129795			
qmof-d57af13	-3.628335268	-6.809510268	3.181175			
qmof-07a7f85	-2.857519359	-6.285645359	3.428126			
qmof-9adcf1a	-3.667425544	-6.827327544	3.159902			
qmof-e2b9aa4	-2.237053853	-5.725571853	3.488518			
qmof-f07eae0	-2.785450016	-5.910665016	3.125215			
qmof-4b12f48	-2.888052449	-6.717590449	3.829538			
qmof-dbd5be4	-2.580730917	-6.761361917	4.180631			
qmof-e628246	-2.183935566	-6.116377566	3.932442			
qmof-25eb644	-2.870251198	-6.035108198	3.164857			
qmof-7344c24	-1.913591196	-6.010835196	4.097244			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-0000295	-1.789690385	-5.604425385	3.814735			
qmof-17eb28a	-3.88549784	-6.23529584	2.349798			
qmof-a46e53c	-3.173636055	-6.080411055	2.906775			
qmof-6bd9402	-3.071236349	-5.549978349	2.478742			
qmof-e53ae74	-2.693052667	-5.975547667	3.282495			
qmof-8f8e33d	-1.920366446	-6.282124446	4.361758			
qmof-0f33589	-2.335138538	-4.828247538	2.493109			
qmof-18924f9	-2.286057541	-5.124832541	2.838775			
qmof-47e505d	-2.239117731	-5.732323731	3.493206			
qmof-1406ccc	-3.021998182	-5.705951182	2.683953			
qmof-01155fc	-3.835382833	-6.671906833	2.836524			
qmof-d65a0ec	-3.019134463	-6.180222463	3.161088			
qmof-fd9f0a1	-2.960873596	-7.046743596	4.08587			
qmof-8e45bb8	-2.973359494	-7.059579494	4.08622			
qmof-219f39d	-2.954824352	-7.048770352	4.093946			
qmof-4f48bfd	-2.910794079	-7.005480079	4.094686			
qmof-d0096f1	-2.967681007	-7.070166007	4.102485			
qmof-d97f36e	-2.969371387	-7.056369387	4.086998			
qmof-f343390	-2.455508951	-5.467652951	3.012144			
qmof-a4aabcfc	-3.831430732	-6.078750732	2.24732			
qmof-542a344	-2.919656109	-6.363353109	3.443697			
qmof-8771d16	-2.455339523	-6.479177523	4.023838			
qmof-284d34c	-2.09135427	-5.06184527	2.970491			
qmof-b1d5255	-3.0720192	-5.4511892	2.37917			
qmof-9fa77bd	-2.553894286	-5.111933286	2.558039			
qmof-360dd73	-3.965090919	-6.275251919	2.310161			
qmof-1eb514c	-3.194236742	-6.201192742	3.006956			
qmof-322e926	-2.988019841	-5.367266841	2.379247			
qmof-47c6882	-3.213223856	-5.984642856	2.771419			
qmof-09f8fe4	-2.035463631	-5.108362631	3.072899			
qmof-9e9806d	-2.940424822	-5.946769822	3.006345			
qmof-4a50fa6	-4.836644023	-7.129758023	2.293114			
qmof-a39fc01	-2.342139309	-6.161992309	3.819853			
qmof-ddf978d	-3.136918143	-6.876747143	3.739829			
qmof-4e4607a	-3.516031373	-6.507940373	2.991909			
qmof-9bd9e21	-3.299592367	-6.441134367	3.141542			
qmof-7981a75	-2.060588864	-4.342030864	2.281442			
qmof-89b132d	-2.692641997	-4.693586997	2.000945			
qmof-aa8159f	-5.675103588	-5.859310588	0.184207			
qmof-c716cfc	-3.053515962	-7.026728962	3.973213			
qmof-7de7cfe	-2.421042514	-6.175564514	3.754522			
qmof-0334ecb	-2.630378797	-6.283752797	3.653374			
qmof-73b0d64	-2.848838285	-7.187577285	4.338739			
qmof-e1d3c58	-2.701591091	-6.705821091	4.00423			
qmof-5d6869e	-3.18956099	-6.34300599	3.153445			
qmof-14eb177	-1.987566428	-5.397042429	3.409476			
qmof-0bbe81c	-1.955129831	-5.181422831	3.226293			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-782ea07	-2.128044493	-5.849505493	3.721461			
qmof-9d5b9ef	-2.830843164	-6.611833164	3.78099			
qmof-99ad091	-4.045135163	-5.729784163	1.684649			
qmof-7e1795a	-2.711944663	-5.314028663	2.602084			
qmof-88c8be3	-3.550779254	-7.159718254	3.608939			
qmof-cafbd5e	-3.765554593	-5.977132593	2.211578	✓		
qmof-c95d01f	-2.851595325	-5.291580325	2.439985			
qmof-b7cf313	-4.420528293	-6.799445293	2.378917			
qmof-c9435a0	-2.026250439	-5.365301439	3.339051			
qmof-85790cf	-3.460378729	-5.894538729	2.43416	✓	✓	
qmof-3ffecec	-3.099788543	-6.245018543	3.14523			
qmof-76b43c3	-3.101693042	-5.254364042	2.152671			
qmof-16e1e21	-3.081913489	-6.243348489	3.161435			
qmof-3af121f	-2.613372434	-4.727047434	2.113675			
qmof-d3f2126	-2.037942805	-6.409844805	4.371902			
qmof-f199346	-4.337174665	-7.113869665	2.776695			
qmof-a487143	-4.487008475	-7.429912475	2.942904			
qmof-001ef83	-2.74694418	-5.19591418	2.44897			
qmof-4be7f74	-2.39879285	-5.44309385	3.044301			
qmof-2cf73c1	-3.719854155	-6.024054155	2.3042	✓		
qmof-0690988	-4.475517425	-4.612506425	0.136989			
qmof-6d6cff3	-4.057361893	-6.272719893	2.215358			
qmof-4033975	-2.274885773	-6.432547773	4.157662			
qmof-35fb0ca	-2.648090501	-6.601385501	3.953295			
qmof-86eb544	-3.140871015	-5.206564016	2.065693			
qmof-e8b1a76	-2.635738004	-6.363340004	3.727602			
qmof-1195366	-3.11892653	-6.63988253	3.520956			
qmof-624a8f0	-2.970313595	-7.096702595	4.126389			
qmof-a8dd8d4	-2.063248052	-5.493813052	3.430565			
qmof-60d01a8	-3.161026835	-6.878320835	3.717294			
qmof-e6da489	-3.256761804	-6.973875804	3.717114			
qmof-fb77b5b	-3.378053203	-7.631691203	4.253638			
qmof-4fe6fe2	-4.578878876	-7.513371876	2.934493			
qmof-e8e4dc5	-2.545927935	-6.688232935	4.142305			
qmof-bb23621	-2.5270709	-6.4994849	3.972414			
qmof-46c4388	-2.301440189	-5.852096189	3.550656			
qmof-739453e	-3.269350991	-6.644459991	3.375109			
qmof-02909bf	-2.665899482	-6.732908482	4.067009			
qmof-56d35fa	-3.255456504	-6.578147504	3.322691			
qmof-bedebedd	-4.132018582	-7.511814582	3.379796			
qmof-957913b	-2.747030001	-6.984198001	4.237168			
qmof-b64c0ab	-2.392770302	-5.749167302	3.356397			
qmof-3aa37a5	-2.852235354	-5.109749354	2.257514			
qmof-511ea8e	-2.003816018	-6.051525018	4.047709			
qmof-7d6a409	-1.600731406	-5.799287406	4.198556			
qmof-9dd4510	-3.036766618	-5.270160618	2.233394			
qmof-be4ff6a	-2.72713776	-4.97327476	2.246137			

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Table S3 – continued from previous page

MOF ID	EA _{HSE06} (eV)	IP _{HSE06} (eV)	E _{gap,HSE06} (eV)	CH ₄	CH ₃ OH	HCOOH
qmof-330637a	-2.703742243	-6.246554243	3.542812			
qmof-315acfe	-2.942857707	-6.445640707	3.502783			
qmof-a3aedc5	-3.116921012	-5.793736012	2.676815			
qmof-3f0e645	-3.445875975	-7.226838975	3.780963			
qmof-32cde2f	-4.102625423	-5.721950423	1.619325			
qmof-08f8729	-3.209460645	-6.173377645	2.963917			
qmof-2a66ccf	-3.272985436	-7.371062436	4.098077			
qmof-d1565a5	-2.856920438	-5.997217438	3.140297			
qmof-e0800cd	-2.629064085	-6.280651085	3.651587			
qmof-638a2cb	-2.773120175	-6.548317175	3.775197			
qmof-be04ff1	-2.491892311	-5.437385311	2.945493			
qmof-e823200	-1.79672112	-5.65194112	3.85522			
qmof-9535ce3	-2.434289457	-5.932091457	3.497802			
qmof-62e81dc	-4.152073834	-6.722417834	2.570344			
qmof-3d85a5e	-2.094211124	-6.291946124	4.197735			
qmof-4629fe7	-2.973688945	-5.109865945	2.136177			
qmof-c80d5aa	-1.576459527	-5.566661528	3.990202			
qmof-6549231	-3.250191857	-7.228701857	3.97851			
qmof-09f59ca	-2.810413267	-5.271006267	2.460593			
qmof-a254fea	-2.262788065	-5.427843065	3.165055			
qmof-468de1c	-3.276461491	-7.281011491	4.00455			
qmof-5990a30	-2.82811932	-5.87763032	3.049511			
qmof-3173783	-2.512671898	-5.976352898	3.463681			
qmof-65e5c0d	-2.181145877	-6.316010877	4.134865			
qmof-a4a3887	-2.581769884	-6.194337884	3.612568			
qmof-2d04c0a	-1.934678865	-6.090192865	4.155514			
qmof-7aca348	-2.775333744	-6.171253744	3.39592			
qmof-2383028	-1.687944668	-6.035853668	4.347909			
qmof-26ddf3f	-3.230694078	-5.411626078	2.180932			
qmof-6c1a7d6	-2.693416832	-5.784668832	3.091252			
qmof-1ee372e	-3.112235926	-5.985989926	2.873754			
qmof-fd9a4f6	-1.989680811	-6.001001811	4.011321			
qmof-35ae1e6	-3.236245844	-5.763016844	2.526771			
qmof-f171323	-2.703564519	-5.105625519	2.402061			
qmof-d184693	-2.792800921	-6.120498921	3.327698			
qmof-4140970	-3.080506978	-5.823828978	2.743322			
qmof-ce84df4	-3.195138223	-6.527825223	3.332687			
qmof-f87c9d1	-3.379692526	-6.459023526	3.079331			
qmof-ec0d951	-2.291671777	-5.789390777	3.497719			
qmof-3f13ba6	-2.2310029	-6.6840739	4.453071			
qmof-6f4c7e7	-3.342607723	-6.574402723	3.231795			
qmof-64af24e	-3.095371051	-6.345132051	3.249761			
qmof-de33c92	-2.996456908	-6.921724908	3.925268			
qmof-15b32d5	-4.366700153	-6.659806153	2.293106			
qmof-e19beef	-2.83575792	-5.48218492	2.646427			
qmof-4f2905b	-2.194445953	-5.824092953	3.629647			
qmof-600a106	-3.139240751	-5.313028751	2.173788			

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Table S3 – continued from previous page

MOF ID	EA_{HSE06} (eV)	IP_{HSE06} (eV)	$\text{E}_{gap,HSE06}$ (eV)	CH_4	CH_3OH	HCOOH
qmof-55d409b	-2.848964913	-6.638752913	3.789788			
qmof-f293ac8	-2.110282824	-4.783651824	2.673369			
qmof-1382eec	-2.990583857	-6.315777857	3.325194			
qmof-1eb97da	-3.648993552	-6.456404552	2.807411			
qmof-f91dbb9	-2.75543135	-5.70765135	2.95222			
qmof-07c2760	-2.928831783	-6.775871783	3.84704			
qmof-55ea716	-2.906997128	-6.261999128	3.355002			
qmof-1cd4692	-1.738748714	-4.616640714	2.877892			
qmof-31183ec	-1.747978611	-4.681063611	2.933085			
qmof-55c83e8	-2.377125305	-6.573008305	4.195883			
qmof-b6395f5	-3.473801917	-6.229171917	2.75537			
qmof-191c12e	-2.806731771	-6.598779771	3.792048			