

ELECTRONIC SUPPLEMENTARY INFORMATION

**A practical computational protocol for photocatalytic reactions beyond ground-state approximations**

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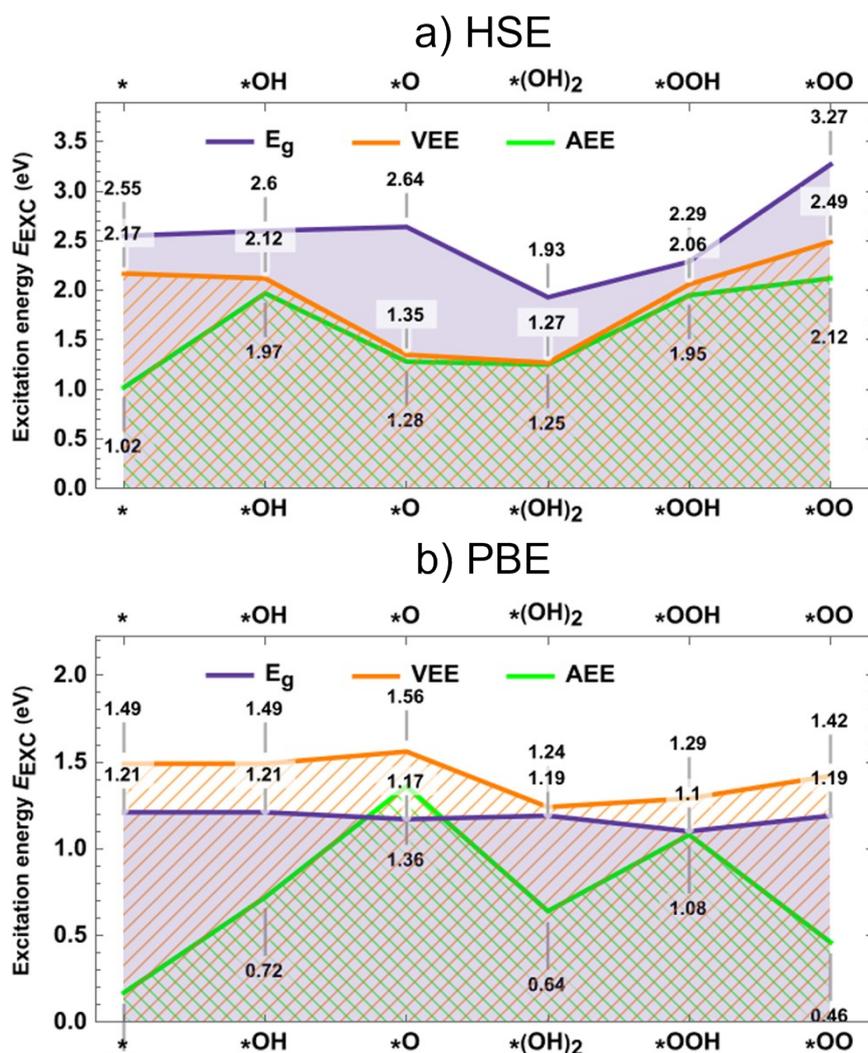
A. Methods

Density functional theory (DFT) calculations were performed using planewave spin-polarized DFT with the Vienna Ab Initio Simulation Package (VASP). PAW basis cutoff was set to 400 eV, according to the PAW library recommendations for the most demanding pseudopotentials used in the study. Values up to 520 eV were evaluated in a convergence test of the \*OOH intermediary (Fig S5). A 2x2 hexagonal supercell ( $\alpha=\beta=90^\circ$   $\gamma=120^\circ$ ,  $c=15$  Å: fixed;  $a=b=14.239$  Å: upon relaxation) of monolayer g-C<sub>3</sub>N<sub>4</sub> was used, containing 56 atoms. DFT-D3 (with Becke-Johnson damping) scheme by Grimme et al. was used to account for van der Waals interactions. 2x2x1  $\Gamma$ -centered kpoint grid was used for relaxations and phonon calculations, and  $\Gamma$  point was used for  $\Delta$ SCF. The structure of the bare catalyst, denoted with "\*" was relaxed in terms of atomic and lattice (xy) degrees of freedom. For all the other intermediaries, only selected atoms were relaxed: Co catalytic site, adsorbate, 3C and 6N atoms in the surrounding of the catalytic site. The atomic/lattice force convergence criterion was set to  $10^{-2}$  eV/Å. The electronic convergence criterion was set to  $10^{-6}$  eV. In "\*", the lowest-energy spin state had 2 unpaired electrons on Co ([Ar]4s<sup>2</sup>d<sup>7</sup>), indicating a +3 oxidation state.

Reaction energetics are determined by calculating the Gibbs free energy differences  $\Delta G$  of subsequent reaction steps. The  $G$  values of different intermediaries are expressed as  $G = E_0 + G(T)$ , the sum of the total energy of the system  $E_0$ , and the finite temperature term  $G(T)$ , which includes zero-point energy, enthalpy and entropy contributions.

$\Delta$ SCF calculations were performed by constraining the desired band occupation structure. Occupancies for spin-up and spin-down channels were kept fixed throughout the calculation. Kohn-Sham orbitals corresponding to g-C<sub>3</sub>N<sub>4</sub> bands ( $-\infty$ , VBM-1] were occupied with 1 electron. The VBM and [CBM+1,  $\infty$ ) were populated with 0 electrons (VBM – g-C<sub>3</sub>N<sub>4</sub> valence band maximum; CBM – g-C<sub>3</sub>N<sub>4</sub> conduction band minimum, Fig S4). States with primarily Co-d character located between VB and CB, the so-called metal midgap states, occupied in a normal SCF calculations, were also occupied in  $\Delta$ SCF. Depending on protocol level, the ground-state geometry was either maintained (Level 1), or re-optimized with the band constraints (Level 2a).

To prevent orbital reordering during  $\Delta$ SCF (required to preserve the non-Aufbau occupation at the selected configuration), an internal setting of LDIAG = False in the INCAR file was used. For velocity friction (ALGO=Damped) and all-bands simultaneous update of orbitals (ALGO=All) algorithms that were used in the study (both ground and excited states), this fixes the occupations of Kohn-Sham orbitals according to the supplied initial setting for both up and down spin states (FERWE, FERDO). Additionally, a VASP source code modification that prevents subspace rotations in the listed ALGO choices was applied. Although the modification was incorporated into official releases of VASP since version 6.3.0, a stable convergence behavior was observed only in an earlier version 5.4.4-patched (6.4.3 was also tested). See Bulancea-Lindvall et al., Phys. Rev. Applied 2024, **22**, 034056 and [https://github.com/defectmrE/DSCF\\_VASP](https://github.com/defectmrE/DSCF_VASP) for more detailed elaboration on the technicalities and demonstrations of VASP  $\Delta$ SCF excited-state computations.



**Fig. S1.**  $E_{\text{EXC}}$  values computed using HSE06+D3(BJ) and PBE+D3(BJ) in different reaction steps: band gap ( $E_g = E_{\text{CBM}} - E_{\text{VBM}}$ ), vertical excitation energy (VEE), and adiabatic excitation energy (AEE). For PBE, the results appear to be not consistent. 1) VEE (the optical gap) is always higher than the fundamental bandgap, which is unphysical; 2) AEE shows extreme variations, including a case when it even exceeds VEE. We attribute this to systematic errors of the PBE functional (self-interaction error, band gap underestimation, etc.) and we urge users to take extreme caution in its use for the study of excited states. We strongly advise the use of the more computational demanding, but reliable HSE hybrid functional for these kinds of studies.

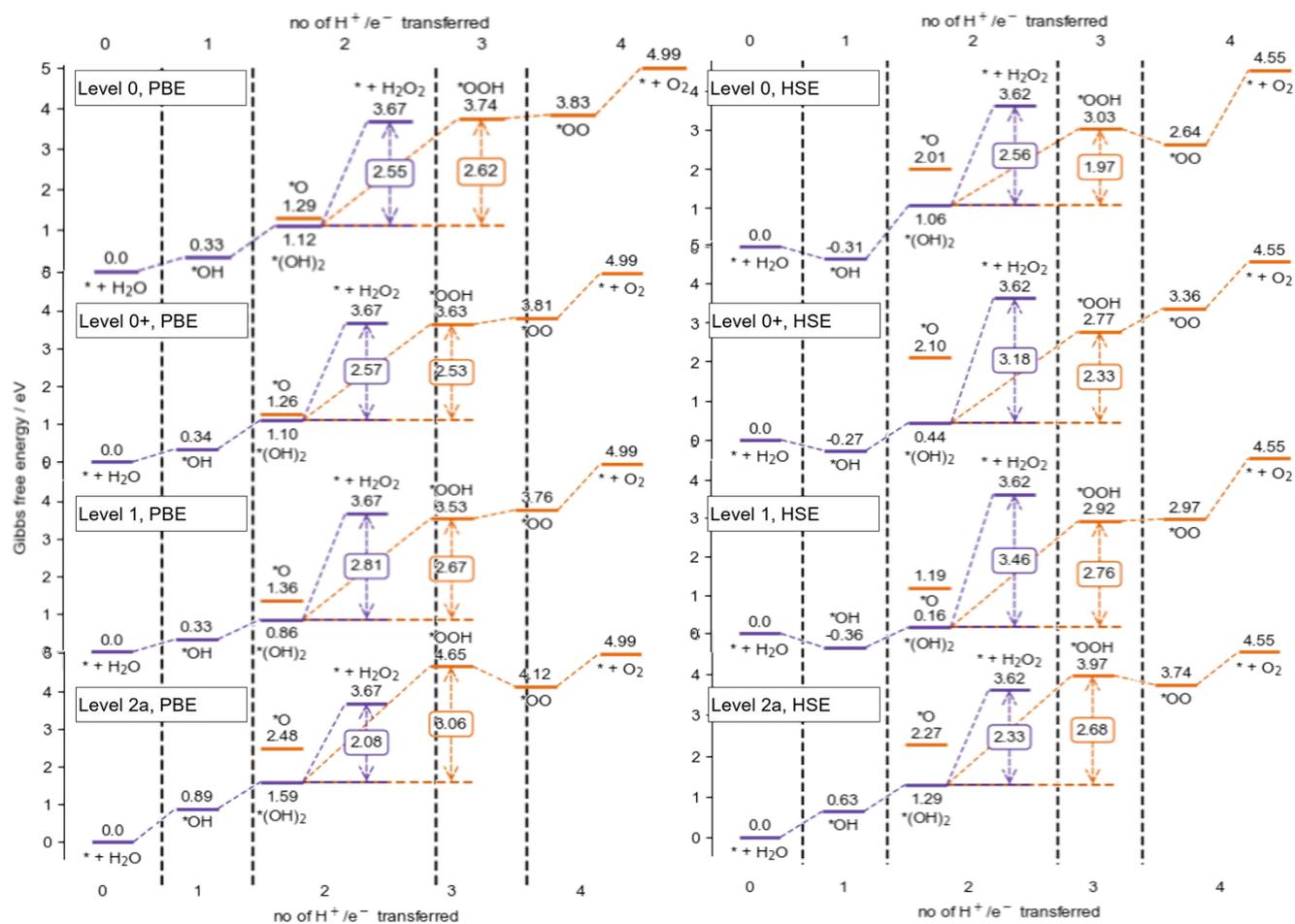


Fig. S2. Gibbs free energy profiles for  $4e^-$  and  $2e^-$  water oxidation reactions for PBE+D3(BJ) and HSE06+D3(BJ).

**Table S1.** Gibbs free energy ( $\Delta G$ ) values along the considered reaction pathways with different functionals and computational framework levels (L0 – Level 0; L0+ - Level 0+; L1 – Level 1; L2a – Level 2a). Values in the brackets are the step-to-step changes for a given reaction intermediary.

4e- water oxidation								
	HSE-L0	HSE-L0+	HSE-L1	HSE-L2a	PBE-L0	PBE-L0+	PBE-L1	PBE-L2a
* + H <sub>2</sub> O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
*OH	-0.31 (-0.31)	-0.27 (-0.27)	-0.36 (-0.36)	0.63 (+0.63)	0.33 (+0.33)	0.34 (+0.34)	0.33 (+0.33)	0.89 (+0.89)
classical *O intermediary:								
*O	2.01 (+2.32)	2.10 (+2.37)	1.19 (+1.55)	2.27 (+1.64)	1.29 (+0.96)	1.26 (+0.92)	1.36 (+1.03)	2.48 (+1.59)
*OOH	3.03 (+1.02)	2.77 (+0.67)	2.92 (+1.73)	3.97 (+1.70)	3.74 (+2.45)	3.63 (+2.37)	3.53 (+2.17)	4.65 (+2.17)
nonclassical *(OH) <sub>2</sub> intermediary:								
*(OH) <sub>2</sub>	1.06 (+1.37)	0.44 (+0.71)	0.16 (+0.52)	1.29 (+0.66)	1.12 (+0.79)	1.10 (+0.76)	0.86 (+0.53)	1.59 (+0.70)
*OOH	3.03 (+1.97)	2.77 (+2.33)	2.92 (+2.76)	3.97 (+2.68)	3.74 (+2.62)	3.63 (+2.53)	3.53 (+2.67)	4.65 (+3.06)
*OO	2.64 (-0.39)	3.36 (+0.59)	2.97 (+0.05)	3.74 (-0.23)	3.83 (+0.09)	3.81 (+0.18)	3.76 (+0.23)	4.12 (-0.53)
* + O <sub>2</sub>	4.55 (+1.91)	4.55 (+1.19)	4.55 (+1.58)	4.55 (+0.81)	4.99 (+1.16)	4.99 (+1.18)	4.99 (+1.23)	4.99 (+0.87)
2e- water oxidation								
	HSE-L0	HSE-L0+	HSE-L1	HSE-L2a	PBE-L0	PBE-L0+	PBE-L1	PBE-L2a
* + H <sub>2</sub> O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
*OH	-0.31 (-0.31)	-0.27 (-0.27)	-0.36 (-0.36)	0.63 (+0.63)	0.33 (+0.33)	0.34 (+0.34)	0.33 (+0.33)	0.89 (+0.89)
*(OH) <sub>2</sub>	1.06 (+1.37)	0.44 (+0.71)	0.16 (+0.52)	1.29 (+0.66)	1.12 (+0.79)	1.10 (+0.76)	0.86 (+0.53)	1.59 (+0.70)
* + H <sub>2</sub> O <sub>2</sub>	3.62 (+2.56)	3.62 (+3.18)	3.62 (+3.46)	3.62 (+2.33)	3.67 (+2.55)	3.67 (+2.57)	3.67 (+2.81)	3.67 (+2.08)
2e- oxygen reduction								
	HSE-L0	HSE-L0+	HSE-L1	HSE-L2a	PBE-L0	PBE-L0+	PBE-L1	PBE-L2a
* + O <sub>2</sub>	4.55	4.55	4.55	4.55	4.99	4.99	4.99	4.99
*OO	2.64 (-1.91)	3.36 (-1.19)	2.97 (-1.58)	3.74 (-0.81)	3.83 (-1.16)	3.81 (-1.18)	3.76 (-1.23)	4.12 (-0.87)
*OOH	3.03 (+0.39)	2.77 (-0.59)	2.92 (-0.05)	3.97 (+0.23)	3.74 (-0.09)	3.63 (-0.18)	3.53 (-0.23)	4.65 (+0.53)
* + H <sub>2</sub> O <sub>2</sub>	3.62 (+0.59)	3.62 (+0.85)	3.62 (+0.70)	3.62 (-0.35)	3.67 (-0.07)	3.67 (+0.04)	3.67 (+0.14)	3.67 (-0.98)

Table S2. Ground state energetics of reaction intermediaries and gaseous species. Zero point energy  $E_{ZPE}$ ; Thermal correction ( $T=298$  K,  $p=1$  atm) to thermodynamic potentials – enthalpy  $H$ , Gibbs free energy  $G$ ; Entropy thermal contribution  $T^*S$ ; Total ground-state energy  $E_0$ ;  $E_{EXC}$  values: band gap  $E_g$ , vertical excitation energy  $VEE$ , adiabatic excitation energy  $AEE$ . All quantities are expressed in eV.  $H_2$ ,  $H_2O$ ,  $H_2O_2$  and  $O_2$  refer to the molecules in gas phase.

(eV)	PBE								HSE							
	$E_{ZPE}$	$\Delta H(T)$	$T^*S$	$\Delta G(T) = \Delta H - TS$	$E_0$	$E_g$	$VEE$	$AEE$	$E_{ZPE}$	$\Delta H(T)$	$T^*S$	$\Delta G(T) = \Delta H - TS$	$E_0$	$E_g$	$VEE$	$AEE$
*	1.36	1.53	0.31	1.22	476.55	1.21	1.49	0.17	1.43	1.58	0.25	1.33	574.47	2.55	2.29	1.02
*OH	1.73	1.97	0.47	1.50	487.55	1.21	1.49	0.72	1.82	2.04	0.41	1.63	588.52	2.60	2.12	1.97
*(OH) <sub>2</sub>	2.12	2.39	0.50	1.90	498.22	1.19	1.24	0.64	2.23	2.48	0.44	2.04	600.97	1.93	1.27	1.25
*OOH	1.81	2.06	0.49	1.57	491.87	1.10	1.29	1.08	1.92	2.18	0.50	1.69	594.71	2.29	2.06	1.95
*O	1.46	1.68	0.41	1.27	482.95	1.17	1.56	1.36	1.53	1.73	0.36	1.37	582.00	2.64	1.35	1.28
*OO	1.50	1.73	0.42	1.31	488.10	1.19	1.42	0.46	1.59	1.84	0.48	1.36	590.85	3.27	3.36	2.12
H <sub>2</sub>	0.27	0.36	0.40	-0.05	-18.54				0.27	0.36	0.40	-0.04	-23.37			
H <sub>2</sub> O	0.56	0.66	0.58	0.08	-14.54				0.59	0.69	0.58	0.11	-17.47			
H <sub>2</sub> O <sub>2</sub>	0.70	0.81	0.71	0.11	-6.77				0.74	0.85	0.70	0.15	-7.83			
O <sub>2</sub>	0.10	0.19	0.63	-0.45	-9.85				0.11	0.20	0.63	-0.44	-13.99			

Table S3. Magnetization of Co along the reaction pathways.

species	Co magnetization (PBE)	Co magnetization (HSE)
*	2.198	2.505
*OH	2.4	2.62
*(OH) <sub>2</sub>	1.247	1.034
*OOH	2.368	2.581
*O	2.521	2.316
*OO	2.231	2.604

Table S4. Benchmark of computed gas-phase thermochemical data against the experimental values.

	PBE	HSE	Exp [1]
	$E_{ZPE}$	$E_{ZPE}$	$E_{ZPE}$
H <sub>2</sub>	0.27	0.27	0.26
H <sub>2</sub> O	0.56	0.59	0.56
H <sub>2</sub> O <sub>2</sub>	0.70	0.74	0.67
O <sub>2</sub>	0.10	0.11	0.10

[1] NIST Computational Chemistry Comparison and Benchmark Database. NIST Standard Reference Database Number 101. Release 22, May 2022, Editor: Russell D. Johnson III. <http://cccbdb.nist.gov/> DOI:10.18434/T47C7Z

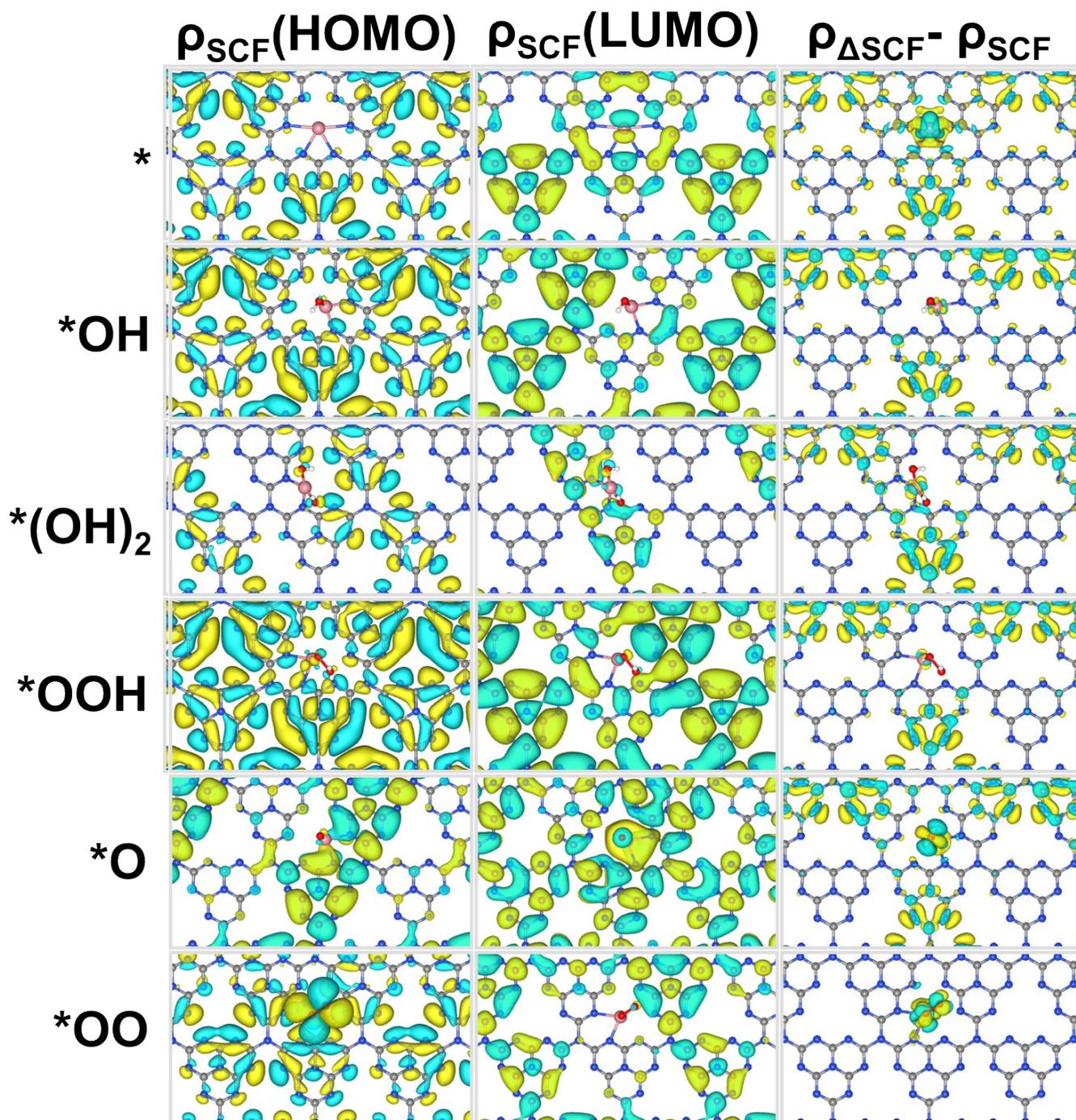


Fig S3. Charge densities corresponding to the projected wavefunctions of self-consistent HOMO (depopulated in  $\Delta\text{SCF}$  level, LUMO (populated), and total charge density difference (isosurface=0.0015) between the  $\Delta\text{SCF}$  and SCF calculations.

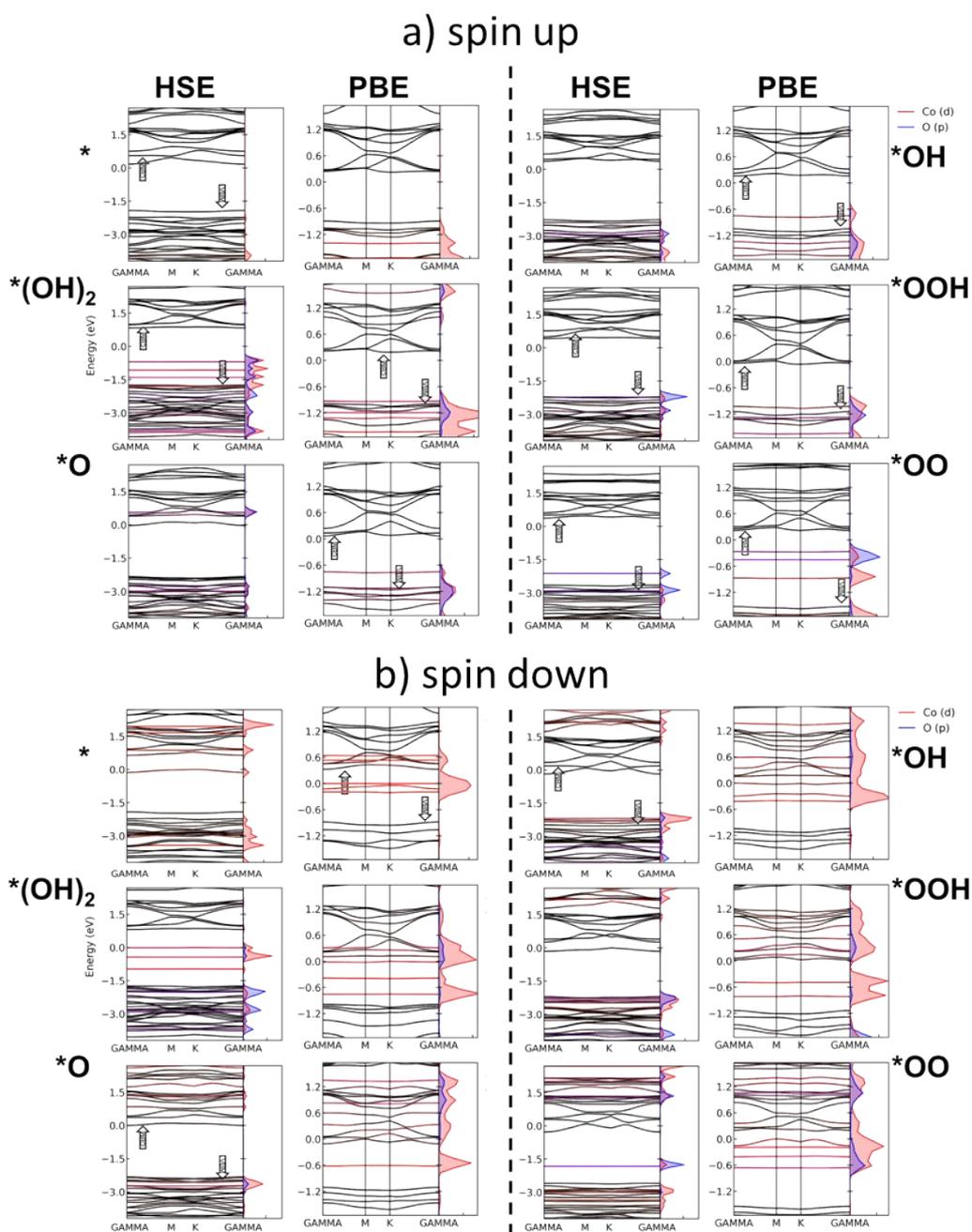


Fig S4. Co(d) and O(p)-projected band structures and density of states of reaction intermediaries. Arrows mark the bands excited with  $\Delta$ SCF. For each intermediary/functional combination, the excitation with the lowest AEE was selected, thus spin polarization may vary between intermediaries.

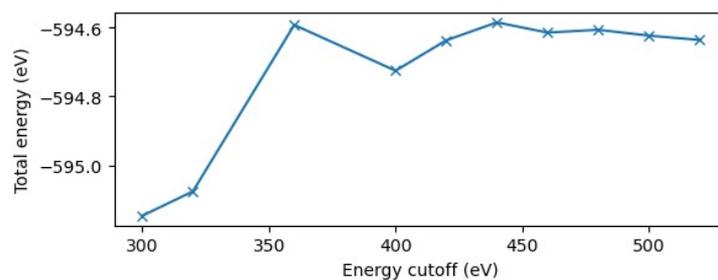


Fig S5. Total energy vs. PAW basis set kinetic energy cutoff, calculated on the \*OOH intermediate with the HSE functional.

## B. Coordinates of optimized structures with the HSE functional, ground state (VASP POSCAR format)

CoCN

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Co C N
1 24 32

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Direct

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1			1
1			1
Direct			
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0.8095919290183815	0.5235392460731418	0.4999998478934344	
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0.8111665079109969	0.6883087253274738	0.4999999853250685	
0.9747229555483159	0.6861648352301586	0.5000002306167417	
0.6450361759561360	0.5262226657565279	0.5039008340537237	
0.8110985585737254	0.8526711655586965	0.5000006526284153	
0.477892588213675	0.5215147330559873	0.6626950624165033	
0.4379769080002518	0.4623539611717149	0.7043972537000371	

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-7.1196551343997641    12.3314751903446478    -0.0000000886142700				
-0.0000000124589763    -0.0000000346580212    14.9999999999999982				
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0.0258594820797384			0.2957727237264791	0.5000001253429431
0.2054901441300530			0.4729278290046040	0.4999999108542283
0.2042788066406871			0.2964683708736189	0.5000000056670473
0.3685866484554055			0.2981096148730771	0.5037421028870597
0.3685685990328764			0.1306826241693955	0.5000000208731947
0.1969927786177053			0.1306820073778212	0.4999996918068206
0.0257104498800302			0.7949704066714958	0.5000001253429431
0.2041196482482022			0.9733607524121766	0.4999999108542212
0.2041396893048594			0.7949692173735556	0.5000000056670615
0.3687167983985802			0.8021981243147991	0.5000002958715442
0.3697843285650748			0.6350613556410636	0.5046528047227525
0.1981843571692679			0.6311362139792465	0.4999996918068135
0.5270704861984754			0.2964695601715519	0.5000001253429289
0.7023162291105365			0.4729278290046040	0.4999999108542283
0.7047929743135342			0.2957715344285390	0.5000000056670615
0.8684369513111889			0.3019939329934687	0.5000002958715584
0.8683889100483100			0.1322263643821913	0.5000000208731876
0.6987162086531526			0.1322257475906170	0.4999996918068064
0.5272672917923131			0.7960541165024253	0.5000001253429360
0.7048392692025232			0.9747999934827476	0.4999999108542212
0.7036665580616841			0.7960529272044852	0.5000000056670615
0.8683612953918143			0.8021981243147991	0.5000002958715442
0.8678312277675175			0.6311368307708207	0.5000000208731805
0.6985619289982168			0.6322464906559375	0.4976141758454560
0.1461632099539898			0.3555149074659667	0.5000000167596497
0.3129367363488811			0.0240525735165349	0.4999998478934131
0.1478994260674398			0.1891611324834059	0.4999993473715776
0.4754885471675365			0.3533122437123524	0.5026536625430751
0.3111811576151453			0.1874828704008280	0.4999999853250756
0.4761424674962598			0.1891632735381066	0.5000002306167204
0.1459934913540266			0.0240518952531588	0.4999996879302984
0.3138306677862488			0.3531099018710151	0.5110930381765044
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0.3143335857329177			0.5259295391212433	0.5146587197224903
0.1463205003922141			0.6861626941754579	0.4999993473715989
0.4764540300306450			0.8526721569205336	0.5000003169783866
0.3120216629307180			0.6883087253274738	0.4999999853250685
0.4762921201378632			0.6875390739673648	0.5020988783454214
0.1488249719259116			0.5235385678097657	0.4999996879302984
0.3129243471378018			0.8532301570660579	0.5000006526284011
0.6442317250647278			0.3555149074659667	0.5000000167596568
0.8128275212997238			0.0244991575674476	0.4999998478934202
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0.8118629416465240			0.1888464376255072	0.4999999853250685
0.9762131659283710			0.1878525916390288	0.5000002306167275
0.6465492912921746			0.0244984793040715	0.4999996879302984
0.8127761380251428			0.3541706865107486	0.5000006526284011
0.6449131279689126			0.8549462277002959	0.5000000167596568
0.8095919290183815			0.5235392460731418	0.4999998478934344
0.6460022176391220			0.6876787788489906	0.4962094543170465
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0.8111665079109969			0.6883087253274738	0.4999999853250685
0.9747229555483159			0.6861648352301586	0.5000002306167417
0.6449737601209620			0.5240380828726785	0.4965065917063640
0.8110985585737254			0.8526711655586965	0.5000006526284153
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CoCN\_OOH

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Co C N O H

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-0.0000000124589763	-0.0000000346580212	14.9999999999999982	
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0.2054901441300530	0.4729278290046040	0.4999999108542283	
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0.3685685990328764	0.1306826241693955	0.5000000208731947	
0.1969927786177053	0.1306820073778212	0.4999996918068206	
0.0257104498800302	0.7949704066714958	0.5000001253429431	
0.2041196482482022	0.9733607524121766	0.4999999108542212	
0.2041396893048594	0.7949692173735556	0.5000000056670615	
0.3687167983985802	0.8021981243147991	0.5000002958715442	
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0.8684369513111889	0.3019939329934687	0.5000002958715584	
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0.7048392692025232	0.9747999934827476	0.4999999108542212	
0.7036665580616841	0.7960529272044852	0.5000000056670615	
0.8683612953918143	0.8021981243147991	0.5000002958715442	
0.8678312277675175	0.6311368307708207	0.5000000208731805	
0.7012066991126531	0.6348390662789214	0.5014190404968630	
0.1461632099539898	0.3555149074659667	0.5000000167596497	
0.3129367363488811	0.0240525735165349	0.4999998478934131	
0.1478994260674398	0.1891611324834059	0.4999993473715776	
0.4733193795822714	0.3533949855703682	0.5025089150375592	
0.3111811576151453	0.1874828704008280	0.4999999853250756	
0.4761424674962598	0.1891632735381066	0.5000002306167204	
0.1459934913540266	0.0240518952531588	0.4999996879302984	
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0.1445755645427553	0.8542711016860665	0.5000000167596568	
0.3142149151394023	0.5244366033359000	0.4947922544147048	
0.1463205003922141	0.6861626941754579	0.4999993473715989	
0.4764540300306450	0.8526721569205336	0.5000003169783866	
0.3120216629307180	0.6883087253274738	0.4999999853250685	
0.4762172479581537	0.6874553436136210	0.4948237424965427	
0.1488249719259116	0.5235385678097657	0.4999996879302984	
0.3129243471378018	0.8532301570660579	0.5000006526284011	
0.6442317250647278	0.3555149074659667	0.5000000167596568	
0.8128275212997238	0.0244991575674476	0.4999998478934202	
0.6465180465743359	0.1878504505843281	0.4999993473715918	
0.9762759716845721	0.3541716778725856	0.5000003169783795	
0.8118629416465240	0.1888464376255072	0.4999999853250685	
0.9762131659283710	0.1878525916390288	0.5000002306167275	
0.6465492912921746	0.0244984793040715	0.4999996879302984	
0.8127761380251428	0.3541706865107486	0.5000006526284011	
0.6449131279689126	0.8549462277002959	0.5000000167596568	
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0.6461012728783615	0.6869014080642586	0.5033720931740291	
0.9751872329739228	0.8532311484278949	0.5000003169783866	
0.8111665079109969	0.6883087253274738	0.4999999853250685	
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CoCN\_OO

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Co C N O  
1 24 32 2

Direct

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0.3681351655955467	0.1301673910743872	0.5000000208731947
0.1969109789600267	0.1301667742828130	0.4999996918068206
0.0254836046303240	0.7945597859138189	0.5000001253429431
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0.2039559137969889	0.7945585966158788	0.5000000056670615
0.3687802694804674	0.8022659875675089	0.5000002958715442
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0.1987368497226996	0.6312061040415031	0.4999996918068135
0.5267884356228123	0.2959213139864474	0.5000001253429289
0.7015331296582588	0.4732564130983263	0.4999999108542283
0.7050026463039814	0.2963265572645213	0.5000000056670615
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0.9764206658871117	0.1883782095909439	0.5000002306167275
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0.8085657094016199	0.5234028394793953	0.4999998478934344
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