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Electronic Supplementary Information

Deformation behavior of amorphous zeolitic imidazolate framework - from supersoft material to the formation of complex multicomponent metallized organic-inorganic alloy

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1. Computational Methods

The deformation simulations are carried out using a combination of two well-tested DFT methods. For structural optimization and elastic properties calculations for both compression and expansion, we us the Vienna *Ab initio* Simulation Package (VASP) [1]. The PAW-PBE potential [2] with generalized gradient approximation (GGA) for the exchange correlation potential is adopted. Limited testing with other potentials on p0 did not show any discernable structure difference at significant increase in computational cost. We used a relatively high energy cutoff of 600 eV, with electronic and ionic force convergence set at 10^{-7} eV and 10^{-5} eV/Å respectively.
We used VASP to obtain stepwise compression, and expansion models of a-ZIF and for their optimization. The stepwise 21 compressed and 19 expanded structures were obtained using the scaling parameter in VASP. To calculate the elastic properties of all compression and expansion points we used VASP. We used the stress (σ_j) and strain (ϵ_i) response analysis scheme [3, 4] to the relaxed structure and then obtained the elastic coefficients (C_{ij}, i, j = 1, 2, 3, 4, 5, 6). To obtain σ_j and C_{ij}, a small strain ϵ (±0.5) % is applied. From the calculated Cij, other mechanical properties such as bulk modulus (K), shear modulus (G), Poisson's ratio (η), Young's modulus (E) are obtained using Voight-Reuss-Hill (VRH) polycrystals approximation [5, 6].

For electronic structure, interatomic bonding, and optical properties calculation, we use the in-house developed orthogonalized linear combination of atomic orbitals (OLCAO) [7] with the structures obtained in the VASP relaxation as input. The bond order (BO) values, the overlap population $\rho_{\alpha\beta}$ between any pair of atoms (α , β) based on Mulliken population analysis [8, 9].

$$\rho_{\alpha\beta} = \sum_{m,\,occ} \sum_{i,j} C^{*m}_{i\alpha} C^{m}_{j\beta} S_{i\alpha,j\beta} \tag{1}$$

In the above equation, $S_{i\alpha,j\beta}$ are the overlap integrals between the i^{th} orbital in the α^{th} atom in the j^{th} orbital in the β^{th} atom. $C^{m}_{j\beta}$ is the eigenvector coefficients of the m^{th} band, j^{th} orbital in the β^{th} atom.

Total bond order density (TBOD) is then obtained normalizing the total BO with cell volume. TBOD is a single metric to access the internal cohesion in the crystal. TBOD consists of its partial component or partial BO density (PBOD) from different types of atomic pairs or groups of atoms in the structural unit. The concept of using the quantum mechanical metric, the TBOD, has been introduced by us in the last several years [10, 11], and applied to many different type of materials to explain their physical properties based on interatomic bonding within the materials [12-16].

The OLCAO method using atomic orbitals in the basis expansion is particularly effective for large complex systems as demonstrated in many recent work in complex organic [17, 18], inorganic [10-14, 16, 19-26], metallic [27-29], biomolecular [30-35] and hybrid [36, 37] materials. In particular, the concept of total bond order density (TBOD) and partial BOD (PBOD) are very instrumental in the explanation of the results and in the provision of new insights based upon interatomic bonding of different types, not restricted to geometric parameters such as BL, bond angle (BA) and coordination shells routinely used in many molecular dynamic simulations.

For calculation of porosity in a-ZIF, the program PLATON [38] is used for all compression and expansion models using "VOID" algorithm. The Van der Waal radius used for this analysis is chosen to be 1.70 Å for C, 1.20 Å for H, 1.55 Å for N and 1.39 Å for Zn with a probe radius of 1.20 Å.

2. Electronic Structure under compression.

The electronic structure of the compressed models are calculated by using the OLCAO method. **Fig. S1** shows the calculated total density of states (TDOS) for each compressed configuration. As can be seen, a-ZIF remains as a large gap insulator with distinctive peaks from different bonding combinations until it reaches the pressure of 51.22 GPa at p19 where it suddenly transforms into a metal with very different TDOS The TDOS for the metallic state has no band gap.

Fig. S2 shows the element-resolved partial DOS (PDOS) of H, C, N, and Zn at points p16 to p21. The PDOS of Zn consists mainly of a narrow peak at -7.85 eV even when the structure as a whole is transformed into a metal at p19. Other PDOS for H, C, and N all lost their distinct peak structures and merge into a broad peak showing the total collapse of the IM molecule in the metallic state.
The PDOS for p20 and p21 are similar to p19 other than a slight decrease in Zn peak and flattening of H, C and N segments. For p19 the PDOS of all atoms do not have a gap implies all kinds of bonding between elements take part in the metallization process. The Femi level is located in a deep valley, also called a pseudo-gap. In crystalline metallic alloys, the presence of pseudo-gap implies crystalline stability. The same concept can be applied to multi-component metallic glasses, or non-crystalline high entropy alloys.

The partial charge (PC) distribution for every atom in a-ZIF model and their evolution with pressure can provide additional insight on its electronic structure. In **Fig. S3**, we show the PC distribution for all 918 atoms for p0, and the 4 points before and at the metallization (p16-p19) with the average PC values for each type atom marked. At p0, the PC for Zn, N, C, and H are +0.926, -0.440, -0.109 and +0.248 electrons respectively. Zn and H are electropositive while N is always electronegative. C can be either electropositive or electronegative depending on the local bonding environment in IM. So, there is a considerable charge transfer from Zn to N through the Zn-N bonds in the framework. The PC for C is most interesting because it starts with two distinct groups. One group has PC close to zero and the other PC falls below zero. The former originates from the C atom bonds to 1 H and 2 N and the other from the C=C double bond in the IM $(C_3N_2H_3)^{-1}$ anion. As pressure increases, the distribution of PC for each atom broadens. In the metallized structure at p19, the Zn atoms are all positively charged as in all other strains but are more scattered in the metallic state with an average value of 0.827 e. Some of N atoms are now positively charged with an average value of -0.399 e and some of the H atoms are now negatively charged with an average value of 0.195 e. These changes have been observed only in the metallic states which shows the complexity of interatomic bonding glassy metals.

The interatomic bonding in a-ZIF under compression is important in revealing the changes in the different types of covalent bonds in the compression process of the rigid framework structure. With only 4 elements in a-ZIF there could be a maximum of 10 different bond pairs depending on the structure under deformation. **Fig. S4** shows a bond order (BO) vs bond length (BL) plot for p0. (Similar plots for other data points are shown in **Fig. S5**). There are four main bonding types in a-ZIF at p0: C–C, C–H, and N–C within the IM and Zn–N bonds that connect the IM in a continuous random network through the Zn atoms. The contribution to the TBOD from different bond pairs is shown in the inset of **Fig. S4**. They are 44.94%, 30.91%, 14.21%, and 9.59% from N-C, C-H, C-C, and Zn-N pairs respectively. The N–H bonds are very far apart at p0 and their contribution to the TBOD is negligible (0.35%). Although the Zn-N bonds contribute to less than 10% of the TBOD, much less than the strong intramolecular covalent bonds within the IM linker, they play a pivotal role in the deformation process. Unlike the strong intramolecular covalent bonds, Zn–N bonds have small deviations in their BL (1.98 Å to 2.04 Å) and BO (0.21e to 0.22e) because the a-ZIF is amorphous phase has well-defined SRO. Thus, the deformation of a-ZIF will be mostly reflected in the changes in the Zn-N bonds as shown in **Fig. S5**.

We have also calculated the optical properties in the form of the complex dielectric function ε (ε_1, ε_2) and the energy loss function ELF($\hbar\omega$) via the OLCAO method. From the zero frequency limit of the real parts of the dielectric function $\varepsilon_1(0)$, we can have a reasonable estimation of the refractive index for the a-ZIF model. These are listed in **Table S4** and complex dielectric function with energy loss function (ELF) for every compression step are shown in **Fig. S6**. In the metallized state the effect of the pseudo-gap is reflected with large absorption at low frequency typical of metals. From the complex dielectric functions we can estimate the bulk Plasmon frequency (ω_p) (listed in **Table S4**) for a-ZIF under pressure. Experimentally, it is easier to measure ω_p using elastic scattering techniques than interband transitions using optical absorption to extract the dielectric function. In **Fig. S7(a)**, we plot the refractive index (*n*) and the Plasmon frequency (ω_p) as a function of strain for compression. The refractive index increases slowly till p19 (2.91). Plasmon frequency increases overall during compression there is a noticeable increase at p10. The ω_p increases to 26.48 eV for p19, which should be easily detectable experimentally.

The atomistic origin of metallization of a-ZIF at the pressure of 51.2 GPa requires special attention for this unexpected phenomenon. We start the discussion with the radial distribution function (RDF) and their partial components (PRDF) of this metallic phase shown in **Fig. S8**. Experimentally it would be very difficult or nearly impossible to resolve the detailed distribution with light atoms, especially the H, and so accurate simulation is the only technique available. The top panel of **Fig. S8** shows the total RDF with prominent peaks marked as A, B, C, A', D and E. Beyond 2.5Å, no structures exist as is true for any amorphous material with no long-range order. The PRDF in **Fig. S8**. shows that the peaks A and A' are from H-H pairs. Peak B is a double peak from N-H and C-H pairs which are impossible to resolve experimentally [21]. Peak C originates from the combination of C-C, N-N and N-C pairs with the latter being a double peak itself, showing two different types of nearest neighbor (NN) N-C pairs. The broad peak D is contributed by Zn-N (a double peak), Zn-C, N-H, and Zn-H (second NN, or SNN) pairs. Lastly, the very broad peak E is mainly from SNN pairs of N-N, N-C, and C-C pairs. Please also note that the y-axes label in **Fig. S8** are not the same for different pairs for easy contrast.

3. Electronic Structure under expansion

The calculated DOS for a-ZIF under expansion is shown in **Fig. S9**. They are quite similar and unremarkable. All the segments in the figure maintain the sharp peaks in the occupied valence band (VB) DOS, which is the same as in p0 because the molecular structure of the IM in a-ZIF remains intact under expansion. The only observable difference is the steady decrease in the band gap (see **Table S6**) as expansion increases and the appearance of defect-like states below the conduction band (CB) edge when the network starts to break. The same unremarkable variations can also be seen in the PC distributions of the selected models under extension in **Fig. S10**. Zn atoms lose charge to N and the PC for C in IM anion can be positive or negative based on the local bonding within the IM molecule.

The BO vs BL distributions for all the expanded a-ZIF models are displayed in **Fig. S11**. As can be seen, the C-C, C-H, N-C, and N-H bonds do not change much under expansion because the IM anion remains intact. The only change is the steady spread of the Zn-N bonds starting at t6, and becoming very obvious at t7 to t10 where the stress vs. strain have two prominent peaks described above that can be attributed to the larger deformation of Zn-N bonds. This spreading of Zn-N bonds continues as the volume increases up to the last data point t19 where the structure has already been fractured. At that point, the Zn-N BL ranges from 1.82 Å to 2.11 Å with corresponding BO ranges decrease from, 0.28 e to 0.18 e. It is observed at t15 there appears Zn-C of BL 2.36 Å and BO of 0.063 e. This is an example when the Zn-N bond breaks the Zn sort of recoil and moves closer to C in the IM molecule. Unlike the compression cases, the other bonds beyond 2.25 Å are negligible including the bonding between N and H.

The calculated optical properties in the form of energy loss function and the complex dielectric functions are shown in **Figure S12**. The variations in the optical properties under expansion is much smaller than those encountered in the compression due to very different deformation behavior and concomitant changes in structures. The calculated optical parameters for expansion are listed in **Table S6**.

4. Supplementary Table

Table S1: Lattice constant, volume (V), strain, stress (pressure P) (GPa), density (ρ), and porosity percentage of all data points under the compression.

Name	Lattice Constant a, b, c (Å) α, β, √	V(Å^3)	Strain%	P(Gpa)	ρ(g/cm^3)	Porosity %
p0	26.253, 23.721, 26.915, 92.69°, 93.79°, 88.89°	16704.1	0.00	0.000	1.071	58.8
p1	25.740, 23.551, 26.697, 91.05°, 94.00°, 90.31°	16141.6	1.14	0.083	1.108	57.4
p2	25.209, 23.066, 26.147, 91.05°, 94.01°, 90.31°	15163.6	3.17	0.206	1.180	54.7
p3	25.062, 22.931, 25.994, 91.05°, 94.01°, 90.31°	14899.1	3.74	0.245	1.201	53.9
p4	24.413, 22.337, 25.321, 91.05°, 94.01°, 90.31°	13771.9	6.23	0.444	1.299	50.2
p5	23.883, 21.852, 24.771, 91.05°, 94.01°, 90.31°	12893.1	8.27	0.552	1.387	46.8
p6	23.352, 21.366, 24.220, 91.05°, 94.01°, 90.31°	12052.5	10.31	0.815	1.484	43.2
p7	22.556, 20.638, 23.394, 91.05°, 94.01°, 90.31°	10861.4	13.37	1.449	1.647	37.2
p8	21.892, 20.031, 22.706, 91.05°, 94.01°, 90.31°	9931.0	15.91	2.288	1.801	31.6
p9	21.494, 19.667, 22.293, 91.05°, 94.01°, 90.31°	9399.1	17.44	3.087	1.903	28.1
p10	21.229, 19.424, 22.018, 91.05°, 94.01°, 90.31°	9055.3	18.46	3.733	1.975	25.7
p11	20.566, 18.817, 21.330, 91.05°, 94.01°, 90.31°	8232.6	21.01	6.114	2.173	19.5
p12	20.300, 18.574, 21.055, 91.05°, 94.01°, 90.31°	7918.0	22.03	7.444	2.259	17.2
p13	19.902, 18.210, 20.642, 91.05°, 94.01°, 90.31°	7461.3	23.56	9.829	2.397	13.7
p14	19.637, 17.967, 20.367, 91.05°, 94.01°, 90.31°	7166.8	24.58	11.740	2.496	11.4
p15	19.371, 17.724, 20.092, 91.05°, 94.01°, 90.31°	6880.2	25.60	14.029	2.600	9.1
p16	18.973, 17.360, 19.679, 91.05°, 94.01°, 90.31°	6464.7	27.13	19.576	2.767	6.5
p17	18.575, 16.996, 19.266, 91.05°, 94.01°, 90.31°	6066.3	28.65	26.210	2.949	4.4
p18	17.912, 16.389, 18.578, 91.05°, 94.01°, 90.31°	5439.3	31.20	42.386	3.289	1.8
p19	17.249, 15.782, 17.890, 91.05°, 94.01°, 90.31°	4857.0	33.75	51.224	3.683	0.3
p20	16.452, 15.054, 17.064, 91.05°, 94.01°, 90.31°	4215.1	36.81	98.392	4.244	0.2
p21	15.922, 14.568, 16.541, 91.05°, 94.01°, 90.31°	3820.2	38.85	146.279	4.682	0.0

Table S2: Lattice constant, volume (V), strain percentage, stress/pressure (GPa), density (ρ) and porosity percentage of all data points under the expansion.

Name	**Lattice Constant a, b, c (Å) α, β, √**	**V(Å^3)**	**Strain%**	**P(Gpa) Stress**	**ρ(g/ cm^3)**	**Porosity %**
p0	26.253, 23.721, 26.915, 92.69°, 93.79°, 88.89°	16704.1	0.00	0.000	1.071	58.8
t1	26.270, 24.037, 27.247, 91.05°, 94.01°, 90.31°	17160.1	0.90	0.059	1.042	59.9
t2	26.668, 24.401, 27.660, 91.05°, 94.01°, 90.31°	17952.0	2.43	0.198	0.996	61.7
t3	26.801, 24.523, 27.798, 91.05°, 94.01°, 90.31°	18221.2	2.94	0.256	0.982	62.2
t4	27.066, 24.765, 28.073, 91.05°, 94.01°, 90.31°	18767.8	3.96	0.393	0.953	63.3
t5	27.332, 25.008, 28.348, 91.05°, 94.01°, 90.31°	19325.3	4.98	0.555	0.926	64.3
t6	27.597, 25.251, 28.623, 91.05°, 94.01°, 90.31°	19893.6	6.00	0.633	0.899	65.3
t7	27.863, 25.494, 28.899, 91.05°, 94.01°, 90.31°	20473.0	7.02	0.93	0.874	66.2
t8	28.393, 25.979, 29.449, 91.05°, 94.01°, 90.31°	21665.3	9.06	0.756	0.826	68.1
t9	28.659, 26.222, 29.724, 91.05°, 94.01°, 90.31°	22278.5	10.07	0.881	0.803	68.9
t10	29.189, 26.708, 30.275, 91.05°, 94.01°, 90.31°	23539.2	12.11	1.019	0.760	70.5
t11	29.720, 27.193, 30.825, 91.05°, 94.01°, 90.31°	24846.7	14.15	0.751	0.720	72.1
t12	30.516, 27.922, 31.651, 91.05°, 94.01°, 90.31°	26897.2	17.21	0.452	0.665	74.3
t13	31.047, 28.407, 32.201, 91.05°, 94.01°, 90.31°	28325.1	19.25	0.315	0.632	75.6
t14	31.843, 29.136, 33.027, 91.05°, 94.01°, 90.31°	30560.3	22.31	0.246	0.585	77.4
t15	32.374, 29.621, 33.577, 91.05°, 94.01°, 90.31°	32113.9	24.34	0.178	0.557	78.5
t16	33.170, 30.350, 34.403, 91.05°, 94.01°, 90.31°	34541.7	27.40	0.159	0.518	80.0
t17	33.700, 30.835, 34.953, 91.05°, 94.01°, 90.31°	36226.4	29.44	0.138	0.494	80.9
t18	34.496, 31.564, 35.779, 91.05°, 94.01°, 90.31°	38854.7	32.50	0.118	0.460	82.2
t19	35.823, 32.778, 37.155, 91.05°, 94.01°, 90.31°	43512.6	37.59	0.109	0.411	84.1

Table S3 Partial bond order density (PBOD) for C–C, C–H, N–C, N–H and Zn–N and total bond order density (TBOD) in unit of electron/(cm)^3 of all data points under compression.

Name	**PBOD C-C**	**PBOD C-H**	**PBOD N-C**	**PBOD N-H**	**PBOD Zn-N**	**TBOD**
p0	0.00403	0.00877	0.01275	0.00010	0.00272	0.02837
p1	0.00417	0.00909	0.01320	0.00010	0.00281	0.02938
p2	0.00444	0.00970	0.01406	0.00011	0.00299	0.03130
p3	0.00452	0.00988	0.01431	0.00011	0.00304	0.03186
p4	0.00490	0.01073	0.01550	0.00012	0.00328	0.03453
p5	0.00524	0.01151	0.01656	0.00013	0.00349	0.03693
p6	0.00562	0.01238	0.01774	0.00014	0.00372	0.03960
p7	0.00626	0.01390	0.01973	0.00015	0.00411	0.04414
p8	0.00688	0.01542	0.02164	0.00017	0.00448	0.04859
p9	0.00730	0.01647	0.02292	0.00018	0.00473	0.05160
p10	0.00760	0.01724	0.02384	0.00019	0.00489	0.05376
p11	0.00842	0.01940	0.02641	0.00022	0.00533	0.05980
p12	0.00879	0.02040	0.02755	0.00023	0.00553	0.06254
p13	0.00937	0.02204	0.02941	0.00025	0.00582	0.06694
p14	0.00982	0.02334	0.03072	0.00027	0.00608	0.07029
p15	0.01027	0.02464	0.03218	0.00028	0.00638	0.07381
p16	0.01101	0.02697	0.03460	0.00031	0.00677	0.07982
p17	0.01190	0.02971	0.03717	0.00037	0.00738	0.08665
p18	0.01355	0.03510	0.04224	0.00051	0.00841	0.10005
p19	0.02895	0.02268	0.02821	0.01295	0.00515	0.10852
p20	0.03431	0.02986	0.03459	0.01604	0.00691	0.13434
p21	0.03963	0.03545	0.03964	0.01958	0.00767	0.15694

Table S4: Calculated Shear modulus (*G*), bulk modulus (*K*), Young's modulus (*E*), Poisson's ratio (*η*), Pugh's modulus ratio ($k = G/K$), Vicker's Hardness (H_V), stress, strain, plasmon frequency (ω_p), refractive index (n) and band gap (Eg) as function under compression.

Name	*G* (GPa)	*K* (GPa)	*E* (GPa)	*η*	*G/K = k*	H_V	Stress (GPa)	Strain %	ω_p (eV)	n	Eg
p0	2.519	8.875	6.903	0.370	0.284	0.423	0.000	0.00	15.63	1.33	4.80
p1	2.492	8.540	6.814	0.367	0.292	0.433	0.083	1.14	16.17	1.35	4.75
p2	2.615	8.100	7.082	0.354	0.323	0.502	0.206	3.17	16.38	1.37	4.65
p3	2.637	7.930	7.122	0.350	0.333	0.523	0.245	3.74	16.42	1.37	4.62
p4	3.075	7.850	8.160	0.327	0.392	0.702	0.444	6.23	16.58	1.40	4.51
p5	3.852	8.789	10.083	0.309	0.438	0.936	0.552	8.27	16.82	1.43	4.55
p6	4.509	10.900	11.888	0.318	0.414	0.980	0.815	10.31	17.16	1.46	4.40
p7	4.683	12.792	12.522	0.337	0.366	0.876	1.449	13.37	17.61	1.51	4.30
p8	6.276	17.304	16.797	0.338	0.363	1.066	2.288	15.91	18.12	1.56	4.14
p9	7.494	21.401	20.133	0.343	0.350	1.161	3.087	17.44	18.47	1.59	3.93
p10	7.779	25.037	21.146	0.359	0.311	1.041	3.733	18.46	21.05	1.62	3.77
p11	10.388	37.640	28.537	0.374	0.276	1.116	6.114	21.01	22.42	1.68	3.20
p12	12.199	45.387	33.588	0.377	0.269	1.214	7.444	22.03	22.36	1.71	3.20
p13	14.851	58.624	41.084	0.383	0.253	1.304	9.829	23.56	23.39	1.75	3.10
p14	16.046	67.349	44.597	0.390	0.238	1.285	11.740	24.58	23.33	1.78	2.73
p15	19.623	79.576	54.397	0.386	0.247	1.541	14.029	25.60	24.08	1.81	3.14
p16	23.158	103.092	64.634	0.396	0.225	1.558	19.576	27.13	24.27	1.86	2.91
p17	31.978	121.234	88.180	0.379	0.264	2.350	26.210	28.65	24.76	1.92	2.36
p18	37.412	191.379	105.370	0.408	0.195	1.868	42.386	31.20	26.11	2.04	2.03
p19	87.693	282.152	238.383	0.359	0.311	5.786	51.224	33.75	26.48	2.91	-
p20	121.507	450.251	334.436	0.376	0.270	6.207	98.392	36.81	27.70	-	-
p21	321.503	547.037	806.510	0.254	0.588	29.952	146.279	38.85	29.44	-	-

Table S5 Partial bond order density (PBOD) for C–C, C–H, N–C, N–H and Zn–N and total bond order density (TBOD) in unit of electron/(cm)^3 of all data points under expansion.

Name	**PBOD**	**PBOD**	**PBOD**	**PBOD**	**PBOD**	**TBOD**
	C-C	**C-H**	**N-C**	**N-H**	**Zn-N**	
p0	0.00403	0.00877	0.01275	0.00010	0.00272	0.02837
t1	0.00393	0.00854	0.01241	0.00010	0.00265	0.02761
t2	0.00375	0.00815	0.01184	0.00009	0.00253	0.02637
t3	0.00370	0.00803	0.01166	0.00009	0.00249	0.02597
t4	0.00359	0.00779	0.01131	0.00009	0.00242	0.02519
t5	0.00349	0.00755	0.01097	0.00008	0.00235	0.02444
t6	0.00339	0.00733	0.01064	0.00008	0.00227	0.02372
t7	0.00329	0.00711	0.01031	0.00008	0.00221	0.02301
t8	0.00311	0.00672	0.00974	0.00008	0.00206	0.02171
t9	0.00303	0.00653	0.00946	0.00007	0.00200	0.02109
t10	0.00286	0.00617	0.00893	0.00007	0.00188	0.01992
t11	0.00271	0.00585	0.00847	0.00007	0.00178	0.01888
t12	0.00250	0.00540	0.00783	0.00006	0.00162	0.01742
t13	0.00238	0.00513	0.00744	0.00006	0.00152	0.01652
t14	0.00220	0.00476	0.00689	0.00006	0.00140	0.01530
t15	0.00209	0.00453	0.00656	0.00005	0.00132	0.01456
t16	0.00195	0.00420	0.00609	0.00005	0.00122	0.01352
t17	0.00186	0.00401	0.00580	0.00005	0.00116	0.01287
t18	0.00173	0.00374	0.00541	0.00004	0.00107	0.01199
t19	0.00154	0.00333	0.00482	0.00004	0.00095	0.01069

Table S6: Calculated Shear modulus (G), bulk modulus (K),Young's modulus (E), Poisson's ratio (η), Pugh's modulus ratio ($k = G/K$), Vicker's Hardness (H_V), stress, strain, plasmon frequency (ω_p), refractive index (n) and band gap (Eg) as function under expansion.

Name	G (GPa)	K (GPa)	E(GPa)	η	$G/K = k$	H_v	Stress (GPa)	Strain %	ω_p(eV)	n	Eg
p0	2.519	8.875	6.903	0.370	0.284	0.423	0.000	0.00	15.63	1.33	4.80
t1	2.414	9.184	6.660	0.379	0.263	0.376	0.059	0.90	15.67	1.33	4.83
t2	2.219	9.491	6.175	0.392	0.234	0.310	0.198	2.43	15.62	1.31	4.83
t3	2.135	9.098	5.941	0.391	0.235	0.303	0.256	2.94	15.61	1.31	4.84
t4	2.394	9.446	6.622	0.383	0.253	0.358	0.393	3.96	15.60	1.30	4.81
t5	2.817	9.204	7.668	0.361	0.306	0.498	0.555	4.98	15.58	1.29	4.75
t6	2.940	9.266	7.976	0.357	0.317	0.535	0.633	6.00	15.56	1.29	4.18
t7	3.039	9.266	8.217	0.352	0.328	0.569	0.923	7.02	15.49	1.28	4.80
t8	2.501	8.216	6.812	0.362	0.304	0.455	0.756	9.06	15.50	1.27	4.03
t9	2.842	8.318	7.654	0.347	0.342	0.568	0.881	10.07	15.51	1.26	4.00
t10	2.992	7.344	7.902	0.321	0.407	0.720	1.019	12.11	15.50	1.25	3.93
t11	2.351	6.494	6.292	0.339	0.362	0.531	0.751	14.15	15.54	1.24	3.97
t12	1.791	5.394	4.839	0.351	0.332	0.397	0.452	17.21	15.47	1.22	4.03
t13	1.377	4.451	3.746	0.360	0.309	0.304	0.315	19.25	15.63	1.21	3.94
t14	1.138	3.551	3.083	0.355	0.320	0.276	0.246	22.31	15.58	1.19	3.83
t15	0.875	3.061	2.398	0.370	0.286	0.202	0.178	24.34	15.54	1.18	3.01
t16	0.521	2.321	1.453	0.396	0.224	0.106	0.159	27.40	15.64	1.17	3.11
t17	0.607	2.157	1.664	0.371	0.281	0.153	0.138	29.44	15.53	1.17	2.98
t18	0.035	0.637	0.103	0.473	0.055	0.003	0.118	32.50	15.65	1.15	3.01
t19	-0.106	0.009	0.103	-1.484	-12.337	-	0.109	37.59	6.44	-	3.16

Table S7: Source of data for figure 8(b). C= calculated, E= experimental.

materials	G (GPa)	K (GPa)	Ref
ZIF-8	1.09	9.23	C [39]
ZIF-4	1.11	1.54	C [40]
ZIF-zni	2.23	15.63	C [41]
UiO-67	5.69	17.15	C [42]
UiO-68	4.18	14.40	C [42]
$C_{10}H_8$, P21=a	4.64	9.98	C [43]
$C_{10}H_8$, P21=c	5.18	10.27	C [43]
$C_{14}H_{10}$, P21=a	3.72	9.86	C [43]
$C_{14}H_{10}$, P21=c	4.05	10.04	C [43]
100 B_2O	7.10	10.50	C [44]
UiO-66-different capping ligands			
Formate	7.07	19.04	C [45]
Hydroxyl	6.87	17.64	C [45]
Chloride	6.82	17.82	C [45]
Brain tissue	0.00	0.05	C [46]
$(CH_3NH_3)_2KBiBr_6$	7.31	14.97	C [47]
$(CH_3NH_3)_2KBiI_6$	5.93	12.91	C [47]
$(CH_3NH_3)_2TlBiBr_6$	7.68	16.24	C [47]
$(CH_3NH_3)_2TlBiI_6$	7.14	14.64	C [47]
α-MUF-10	1.30	6.80	C [48]
β-MUF-10	3.20	11.70	C [48]
Dibenzyl	2.40	5.10	E [49, 50]
Iododurene	2.80	5.80	E [49]
Benzene (240 K)	2.00	4.80	E [49, 50]
Benzophenone	2.60	5.40	E [49, 50]
Anthracene	3.20	7.60	E [49, 50]
Hexamine	6.10	7.70	E [49]
Naphthalene	3.00	5.60	E [49]
p-DCBP	3.20	7.40	E [49]
Tolan	3.00	4.40	E [49]
340 H_2O-vol NOT fixed	5.70	11.99	C[51]
340 H_2O-vol fixed	5.67	11.01	C[51]
$Co_{54}N_{216}C_{324}H_{324}$	7.36	17.01	C[51]
$Zn_{54}N_{324}C_{216}H_{216}$	4.04	14.14	C[51]
$Li_{27}B_{27}N_{324}C_{216}H_{216}$	5.61	11.90	C[51]
GeS_2	5.87	8.48	C[51]

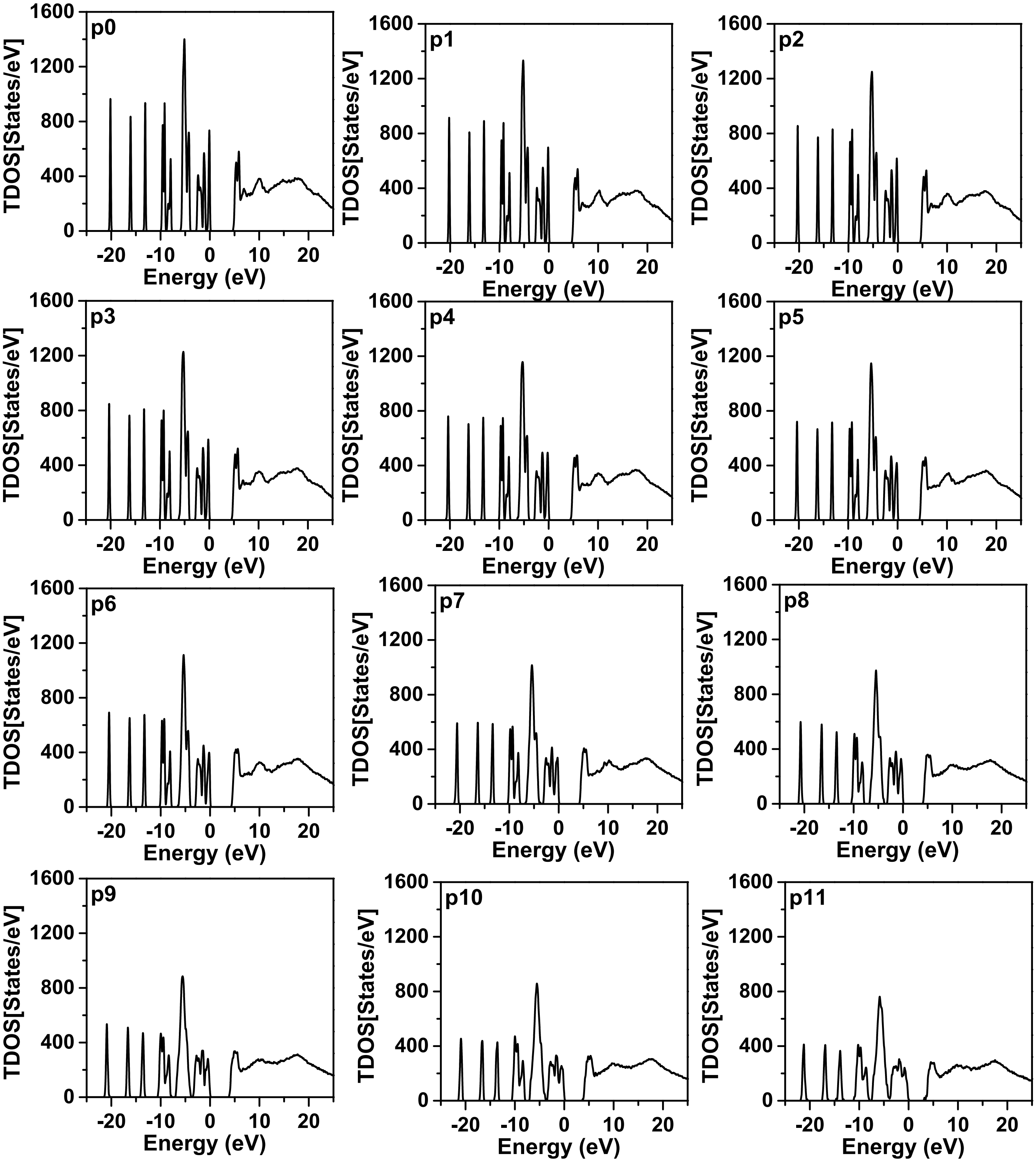
Materials	G(GPa)	K(GPa)	Ref
$GeSe_2$	3.96	6.97	C[51]
As_2S_3	6.96	13.10	C[51]
As_2Se_3	4.91	7.57	C[51]
As_4Se_4	2.17	3.16	C[51]
Ge_4Se_9	4.32	6.50	C[51]
TlBr	7.58	22.46	E [52]
TlCl	7.58	23.56	E [52]
CsBr	7.50	13.01	E [52]
CsI	6.24	12.67	E [52]
KBr	5.08	15.03	E [52]
KCl	6.24	17.36	E [52]
KI	6.20	12.00	E [52]
Egg white			
Cross-linked crystal	0.70	4.51	E [53]
Non-Cross-linked crystal	1.17	4.20	E [53]
Non-Cross-linked crystal	2.64	9.46	E [53]
$Sr_{60}Mg_{18}Zn_{22}$	7.71	14.60	E [54]
$Sr_{60}Li_5Mg_{15}Zn_{20}$	7.02	16.10	E [54]
$Sr_{60}Mg_{20}Zn_{15}Cu_5$	7.76	15.30	E [54]
$Zn_{20}Ca_{20}Sr_{20}Yb_{20}Li_{11}Mg_9$	6.30	12.00	E [55]
Breakaway glass	1.40	3.90	E [55]
Glassy sulfur (at 0 C)	2.10	7.90	E [56]
$Se_{70}Ge_3$	6.20	11.70	E [55]
Amorphous Se	3.50	9.90	E [55]
ZIF-8	1.10	7.75	E [39]
100 B_2O	6.90	12.10	E [57]
RbBr	6.60	13.80	E [58]
RbI	5.10	11.20	E [58]
Stishovite	0.00	0.00	E [59]
B_2O_3 glass	6.10	13.20	E [60]
As_2O_3 glass	4.50	10.90	E [60]
$Ge_{18.2}Sb_{18.2}Se_{63.6}$	7.97	15.21	E [61]
$Ge_{23.3}Sb_{3.3}Se_{73.3}$	6.57	13.44	E [61]
$Ge_{13.3}Sb_{3.3}Se_{83.5}$	5.49	11.76	E [61]
Se	4.63	11.45	E [61]
$Se_{83}Te_{17}$	4.60	11.47	E [61]
$Ge_{13.3}Sb_{13.3}Se_{73.4}$	7.08	13.81	E [61]
$Ge_{23.3}Sb_{13.3}Se_{63.7}$	7.96	14.73	E [61]
$Ge_{25}Sb_{10}Se_{65}$	7.28	13.61	E [61]
$Ge_{26.7}Sb_{6.7}Se_{66.7}$	7.47	13.27	E [61]
$Ge_{16.7}Sb_{16.7}Se_{66.7}$	7.99	14.93	E [61]
$Ge_{20}Sb_{10}Se_{70}$	6.98	13.25	E [61]
$Ge_{16.7}Sb_{6.7}Se_{76.7}$	6.55	11.93	E [61]

materials	G (GPa)	K (GPa)	Ref
$Ge_{3.3}Sb_{3.3}Se_{93.4}$	4.12	10.21	E [61]
$Ge_{6.7}Sb_{6.7}Se_{86.6}$	5.60	13.02	E [61]
$Ge_{10}Sb_{10}Se_{80}$	5.89	11.87	E [61]
$Ge_{6.7}Sb_{16.7}Se_{76.7}$	6.94	14.06	E [61]
$Ge_{30}Se_{70}$	6.44	12.23	E [61]
$Ge_{20}Se_{80}$	5.65	11.45	E [61]
$Ge_{10}Se_{90}$	4.29	9.39	E [61]
$Ge_{25}Se_{75}$	6.67	12.53	E [61]
Argon	1.4	1.8	E [50]
Cesium	1.6	2.2	E [50]
Rubidium	1.9	2.7	E [50]
Potasium	2.65	3.6	E [50]
Benzene	3.25	4.6	E [50]
Dibenzyl	3.45	4.8	E [50]
Tolane	3.45	4.1	E [50]
Sodium	3.6	4.4	E [50]
$Ge_{22}Se_{78}$	6.30	12.48	E [61]
$Ge_{13.3}Sb_{8.9}Se_{61.1}As_{4.4}Te_{12.3}$	7.16	14.04	E [61]
$Ge_{16.7}Sb_{11.1}Se_{55.6}As_{5.6}Te_{11.1}$	7.18	14.38	E [61]
$Ge_{20}Sb_{6.7}Se_{58.3}As_{3.3}Te_{11.7}$	7.43	15.65	E [61]
$Ge_{10}Sb_{13.3}Se_{58.3}As_{6.7}Te_{11.7}$	7.92	15.70	E [61]
$Ge_{16.7}Sb_{4.5}Se_{63.9}As_{2.2}Te_{12.8}$	6.56	13.43	E [61]
$Ge_{3.3}Sb_{2.2}Se_{77.8}As_{1.1}Te_{15.6}$	4.83	11.72	E [61]
$Ge_{6.7}Sb_{4.5}Se_{72.2}As_{2.2}Te_{14.4}$	5.67	13.35	E [61]
$Ge_{13.3}Sb_{2.2}Se_{69.4}As_{1.1}Te_{13.9}$	5.67	13.18	E [61]
$Ge_{10}Sb_{6.7}Se_{66.7}As_{3.3}Te_{13.3}$	6.41	13.58	E [61]
$Ge_{6.7}Sb_{11.1}Se_{63.9}As_{5.6}Te_{12.8}$	7.39	15.05	E [61]
$Ge_{20}Se_{66.7}Te_{13.3}$	6.26	13.27	E [61]
$Ge_{10}Se_{75}Te_{15}$	5.73	12.86	E [61]
$Ge_{3.3}Sb_{15.5}Se_{61.1}As_{7.7}Te_{12.2}$	7.73	16.11	E [61]
$Ge_{3.3}Sb_{8.8}Se_{69.4}As_{4.4}Te_{13.9}$	6.54	14.93	E [61]
$Sb_{6.7}Se_{75}As_{3.3}Te_{15}$	5.66	13.05	E [61]
$Ge_{22}Se_{64.7}Te_{13.3}$	6.28	12.93	E [61]
$Ge_{3.3}Sb_{3.3}Se_{56}Te_{37.4}$	5.78	12.82	E [61]
$Ge_{6.7}Sb_{6.7}Se_{52}Te_{34.6}$	6.63	13.66	E [61]
$Ge_{13.3}Sb_{3.3}Se_{50.1}Te_{33.4}$	6.75	13.46	E [61]
$Ge_{10}Sb_{10}Se_{48}Te_{32}$	7.09	15.92	E [61]
$Ge_{20}Se_{48}Te_{32}$	6.99	13.79	E [61]
$Ge_{10}Se_{54}Te_{36}$	6.10	12.78	E [61]
$Se_{60}Te_{40}$	5.38	12.74	E [61]
Benzophenone	3.75	5.15	E [50]
Naphthalene	4.25	5.4	E [50]
Anthracene	4.7	6.9	E [50]
Stilbene	4.8	6.7	E [50]

materials	G (GPa)	K (GPa)	Ref
Ice	4.9	7.3	E [50]
Acenaphithene	4.95	6.6	E [50]
Terpin Monohydrate	5.05	7.1	E [50]
Hexamethylenetetramine	6.95	8.4	E [50]
Argon	1.4	1.8	E [50]
Cesium	1.6	2.2	E [50]
Rubidium	1.9	2.7	E [50]
Potasium	2.65	3.6	E [50]
Benzene	3.25	4.6	E [50]
Dibenzyl	3.45	4.8	E [50]
Tolane	3.45	4.1	E [50]
Sodium	3.6	4.4	E [50]

5. Supplementary Figures

Fig. S1 Total density of states of all data points under compression.



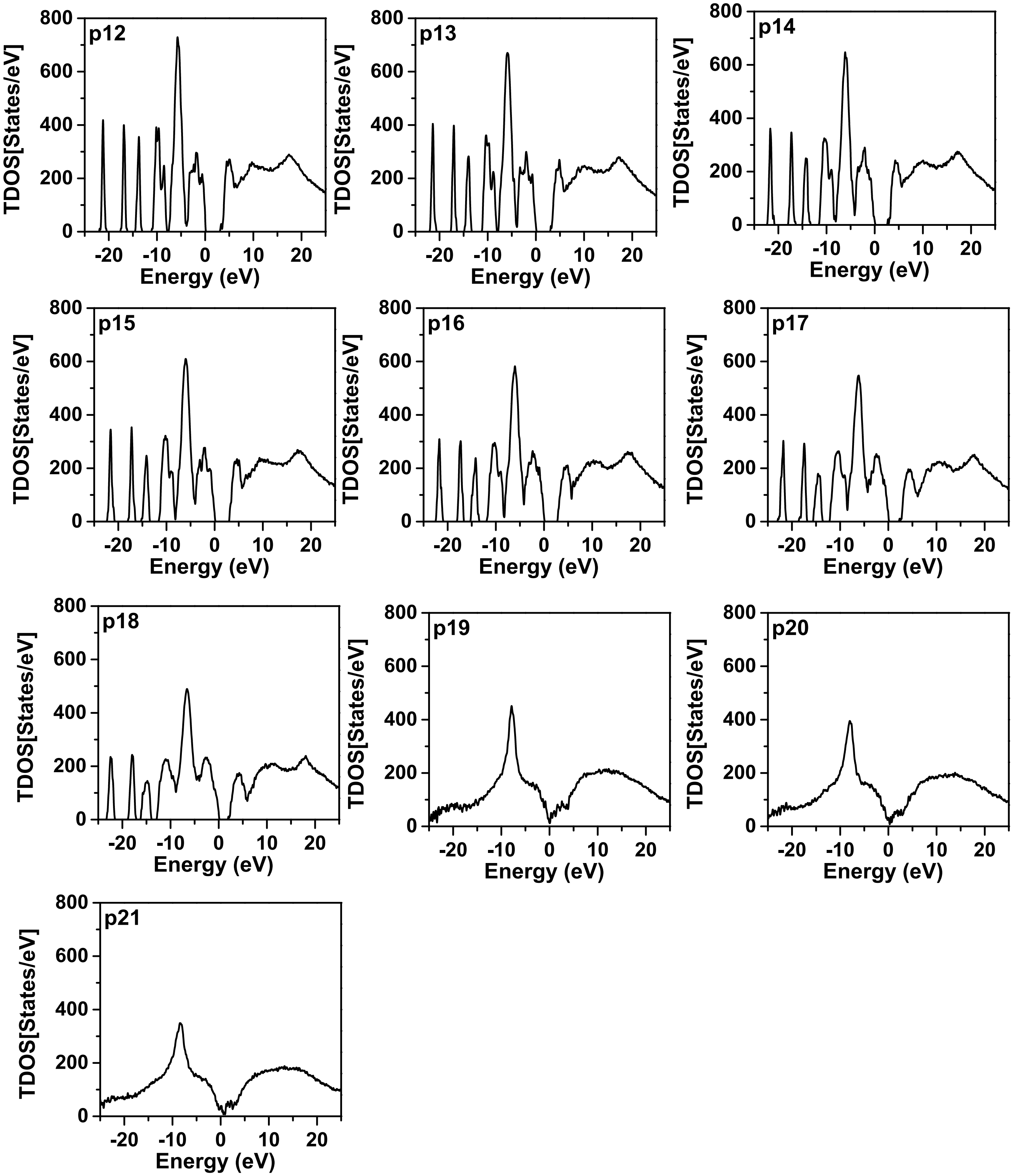

p12
p13
p14
p15
p16
p17
p18
p19
p20
p21
TDOS[States/eV]
Energy (eV)

Fig. S2 Selected partial density of states for compression.

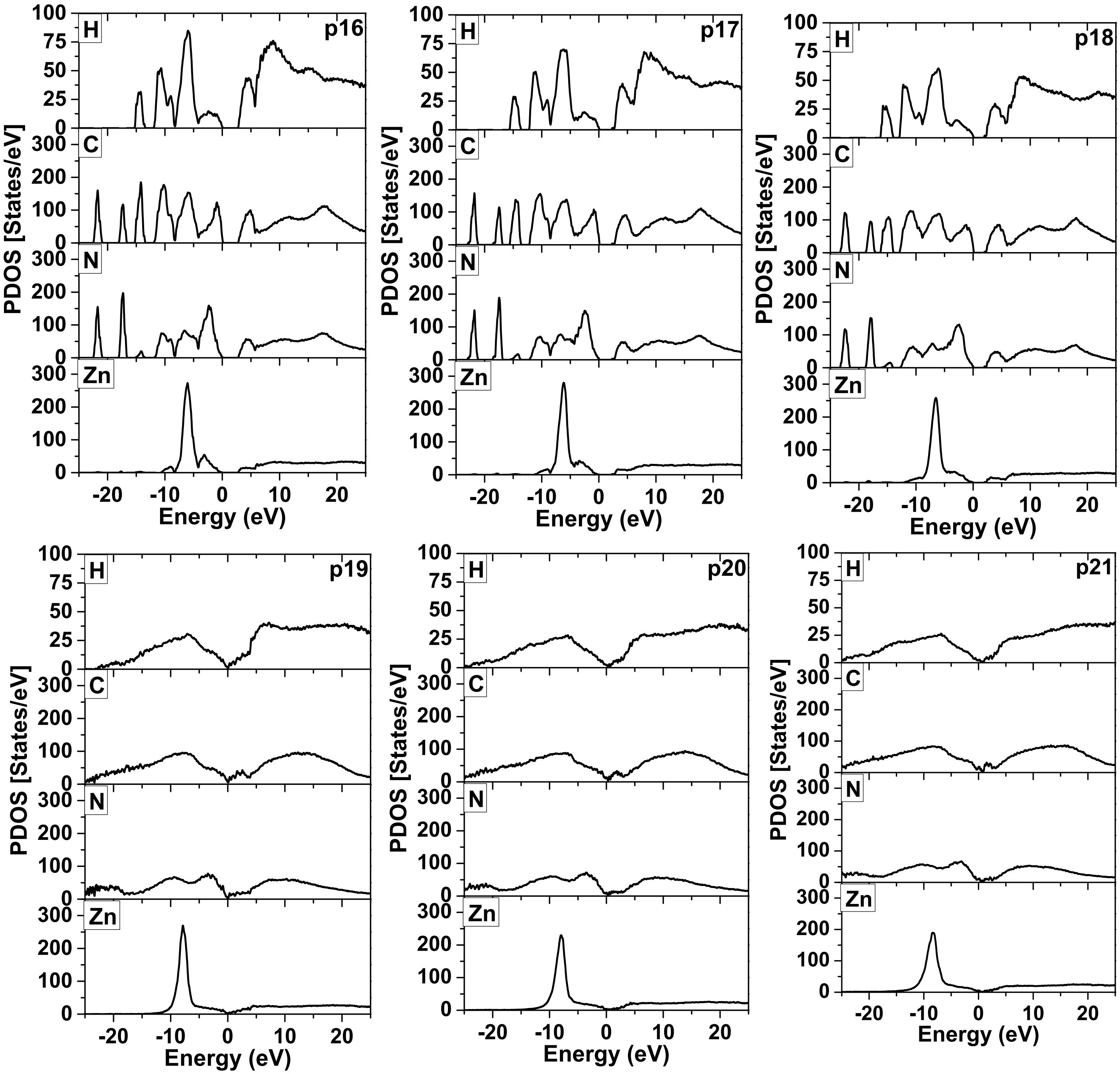


Fig. S3 Selected partial charge distribution for compression.

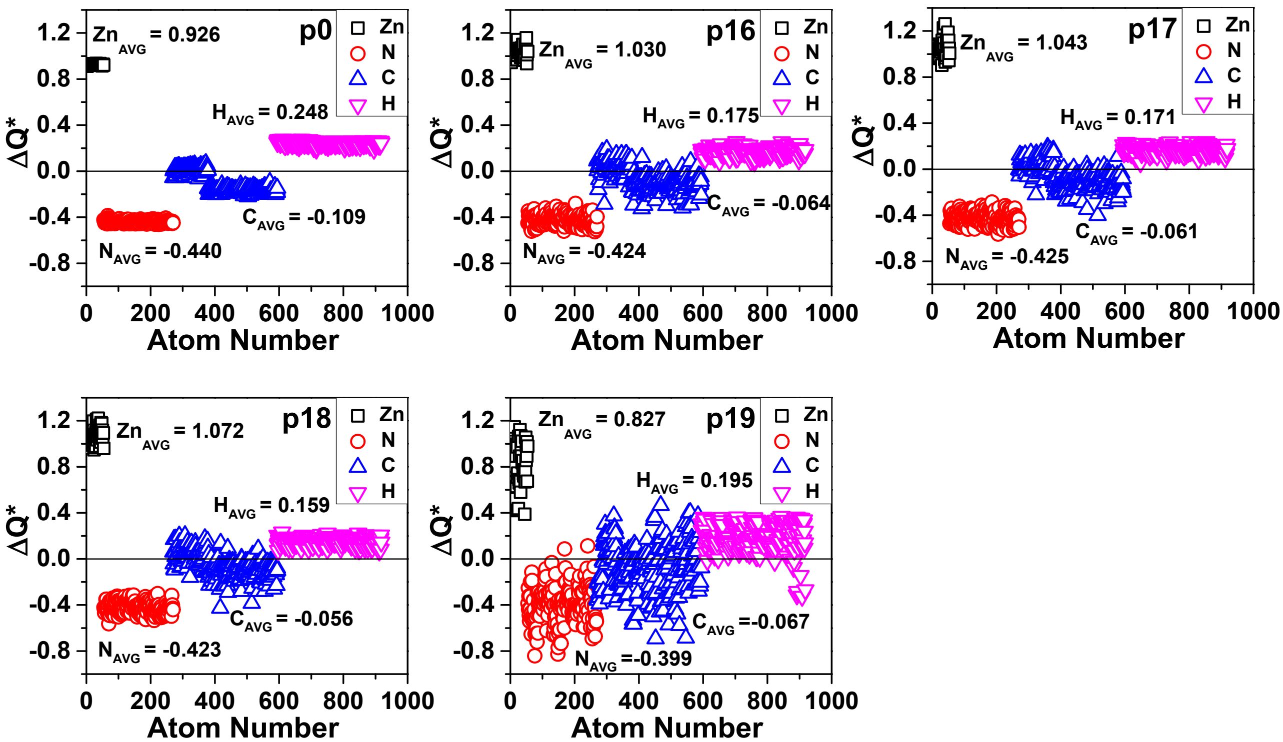


Fig. S4. Bond order (e$^-$) vs. bond length (Å) for a-ZIF for p0. Inset: % contribution to the total bond order density from different bonds.

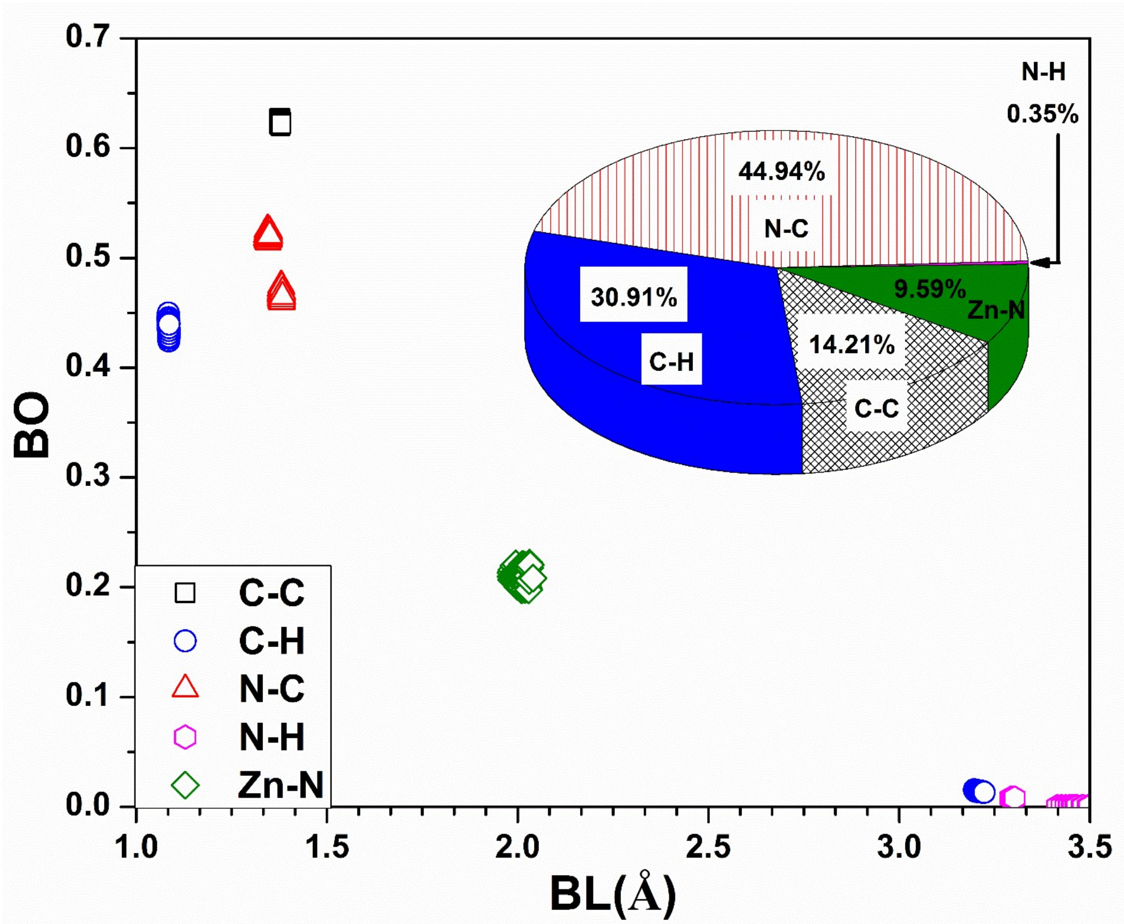
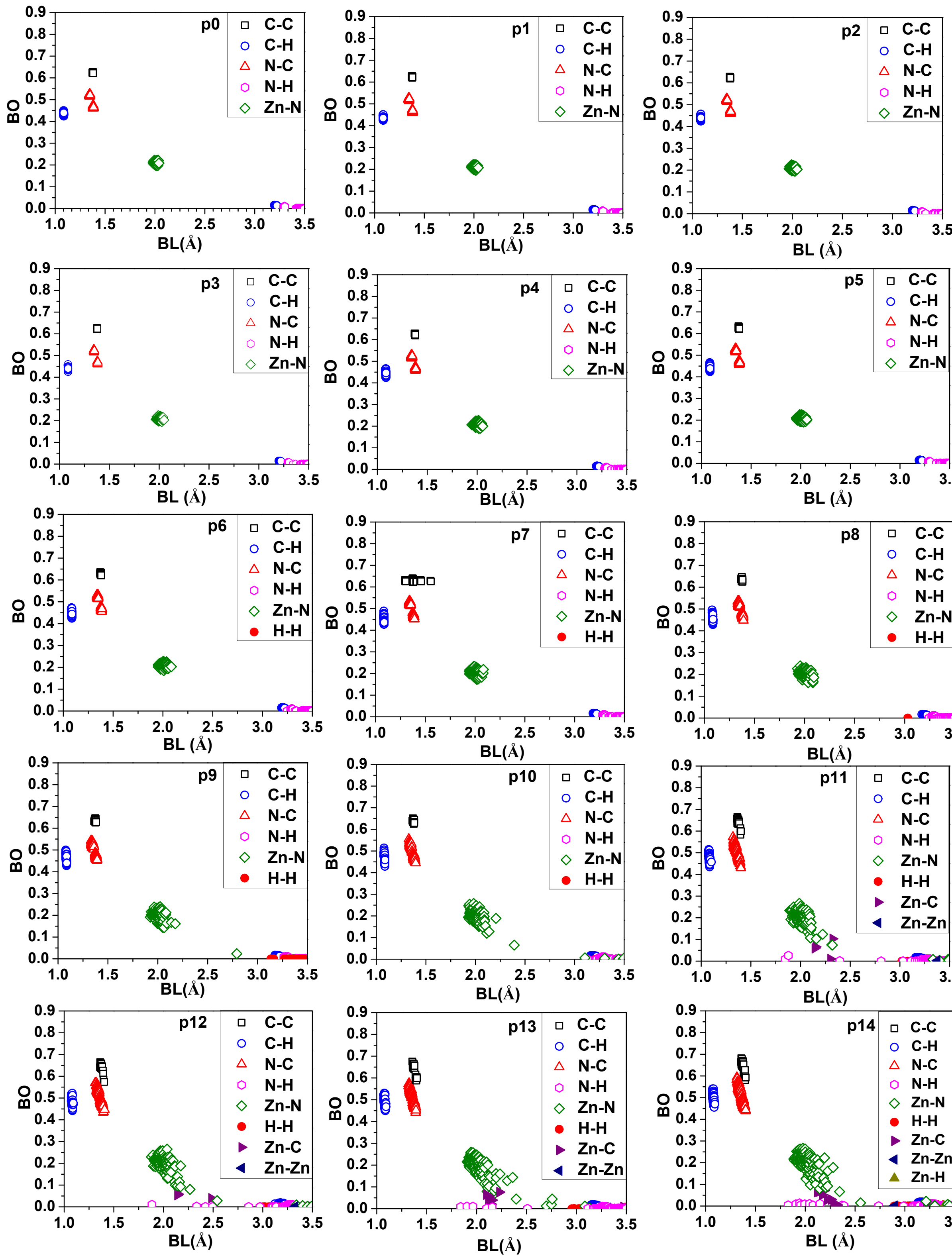


Fig. S5 Bond order (e^-) vs. bond length (Å) of all data points under compression.



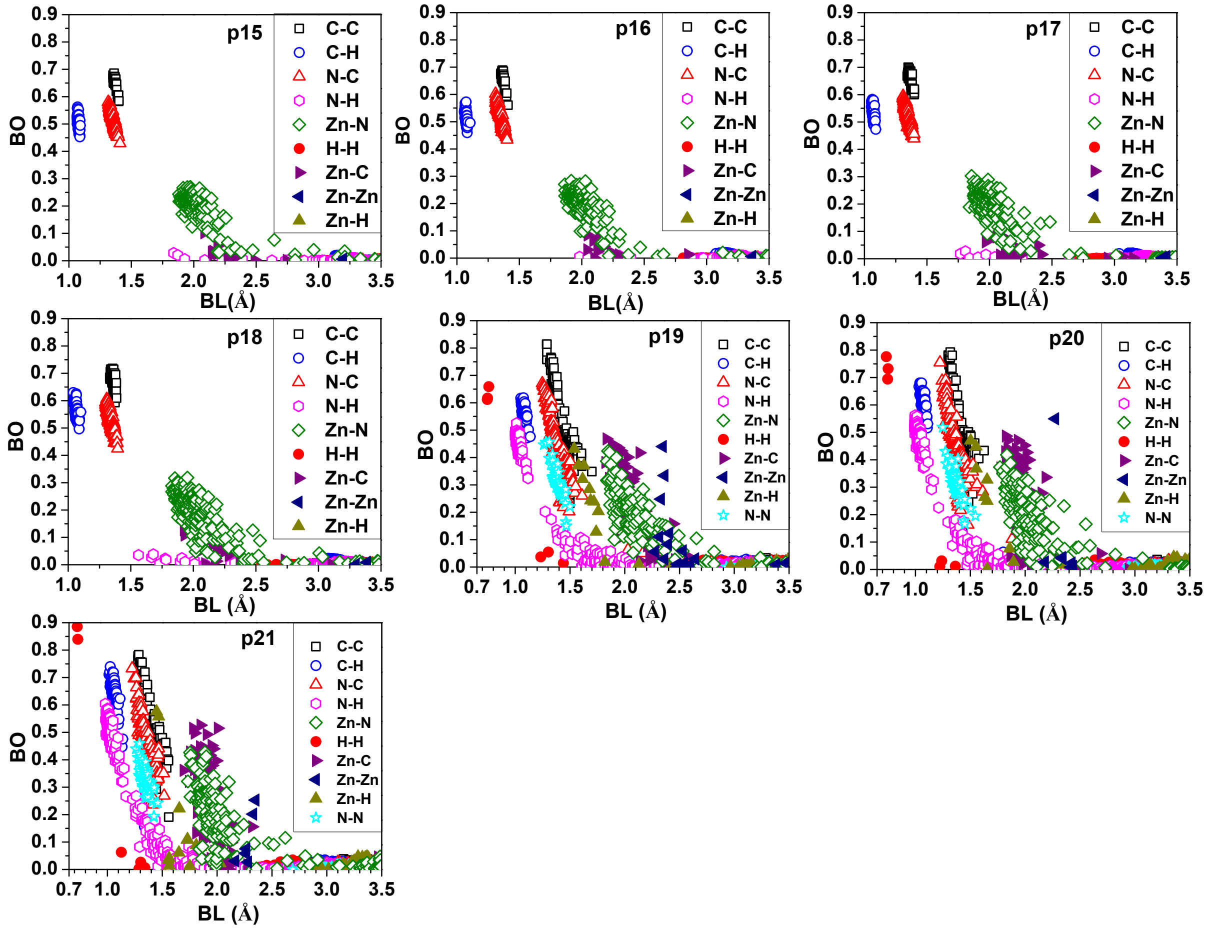
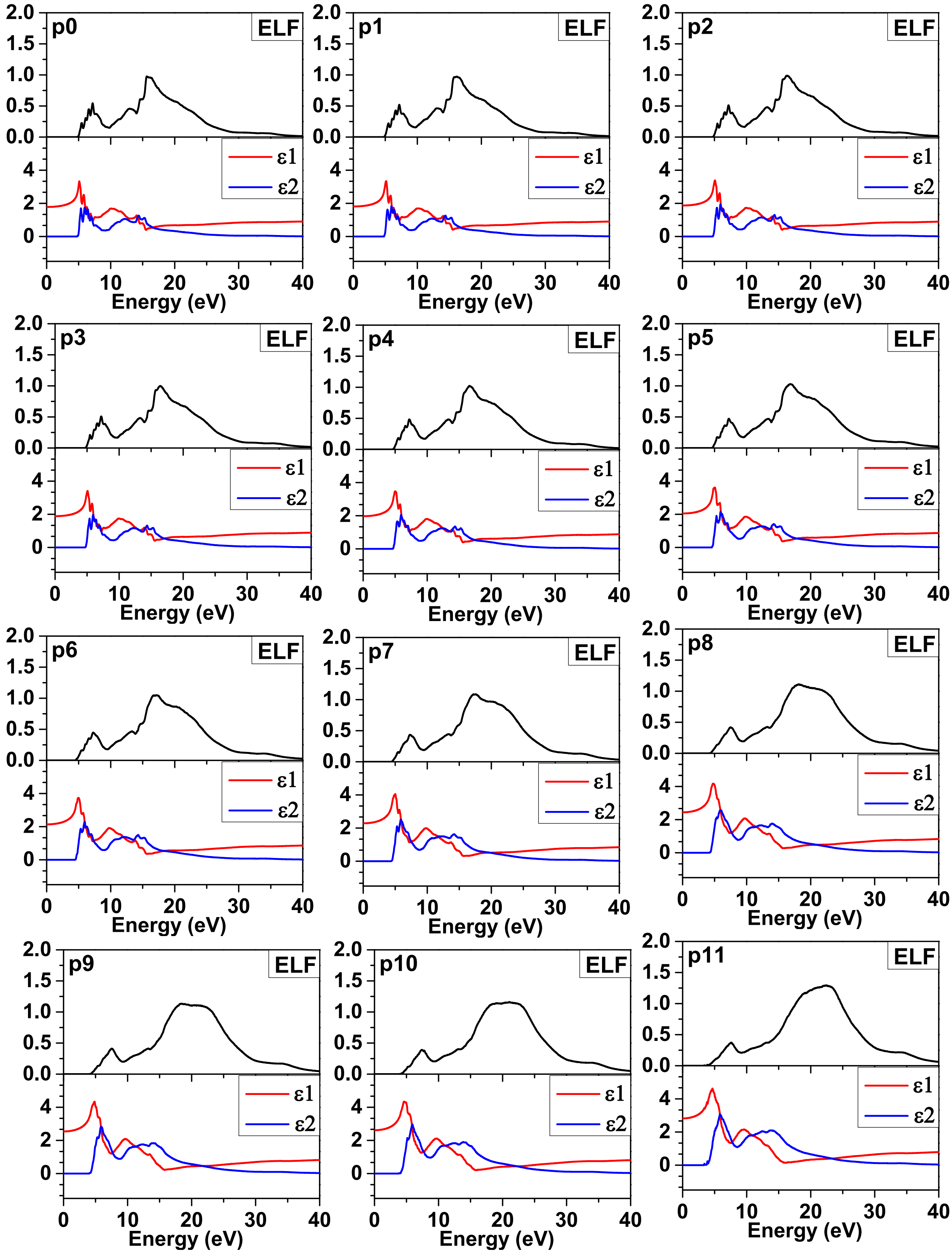

p15
p16
p17
p18
p19
p20
p21
BO
BL(Å)
BL (Å)
C-C
C-H
N-C
N-H
Zn-N
H-H
Zn-C
Zn-Zn
Zn-H
N-N

Fig. S6 Optical properties of all data points under under compression.


p0
ELF
ε1
ε2
Energy (eV)
p1
p2
p3
p4
p5
p6
p7
p8
p9
p10
p11

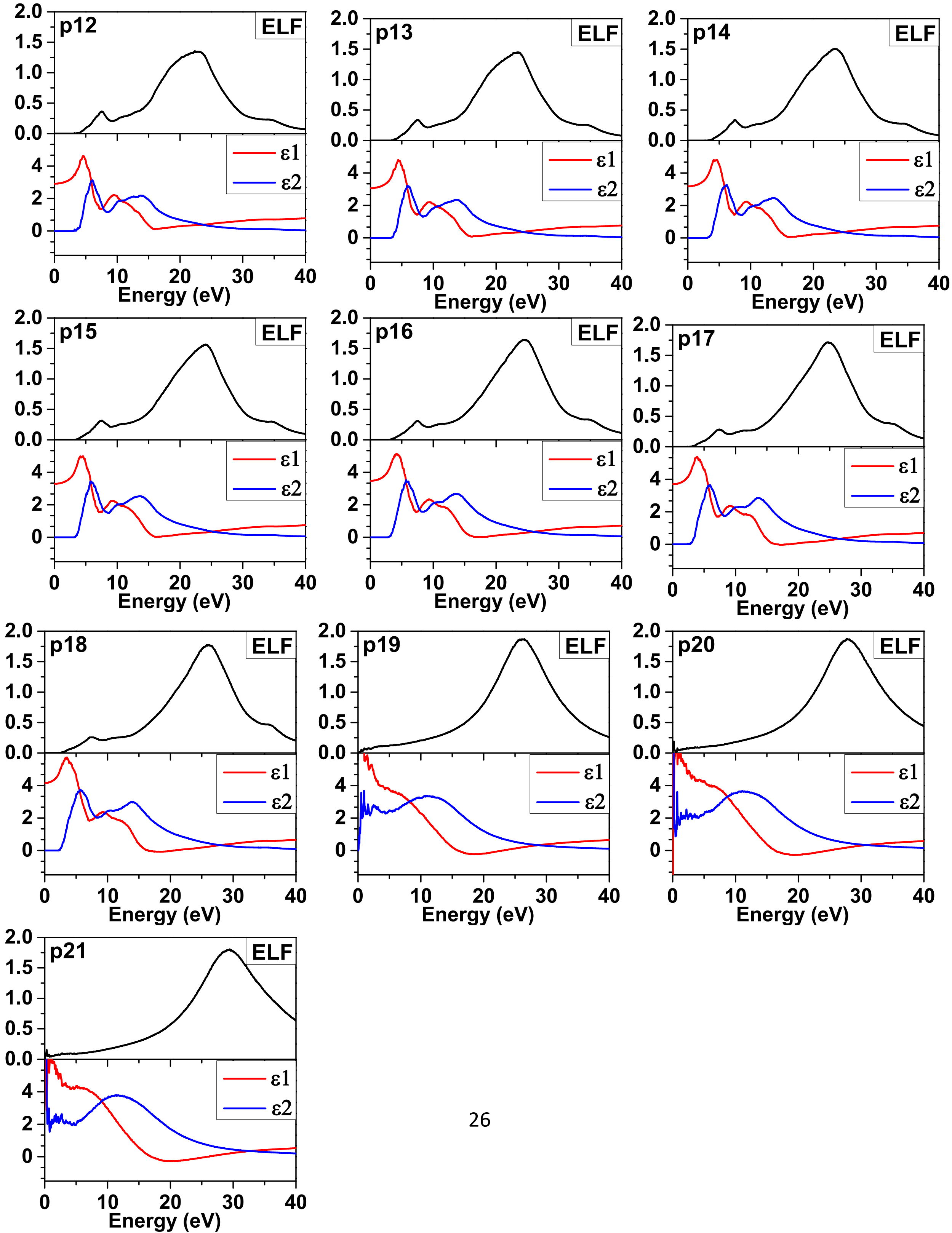

p12
p13
p14
p15
p16
p17
p18
p19
p20
p21
ELF
ε1
ε2
Energy (eV)

Fig. S7 Plasmon frequency (ω_p) and refractive index (n) vs. strain for **(a)** compression and **(b)** expansion.

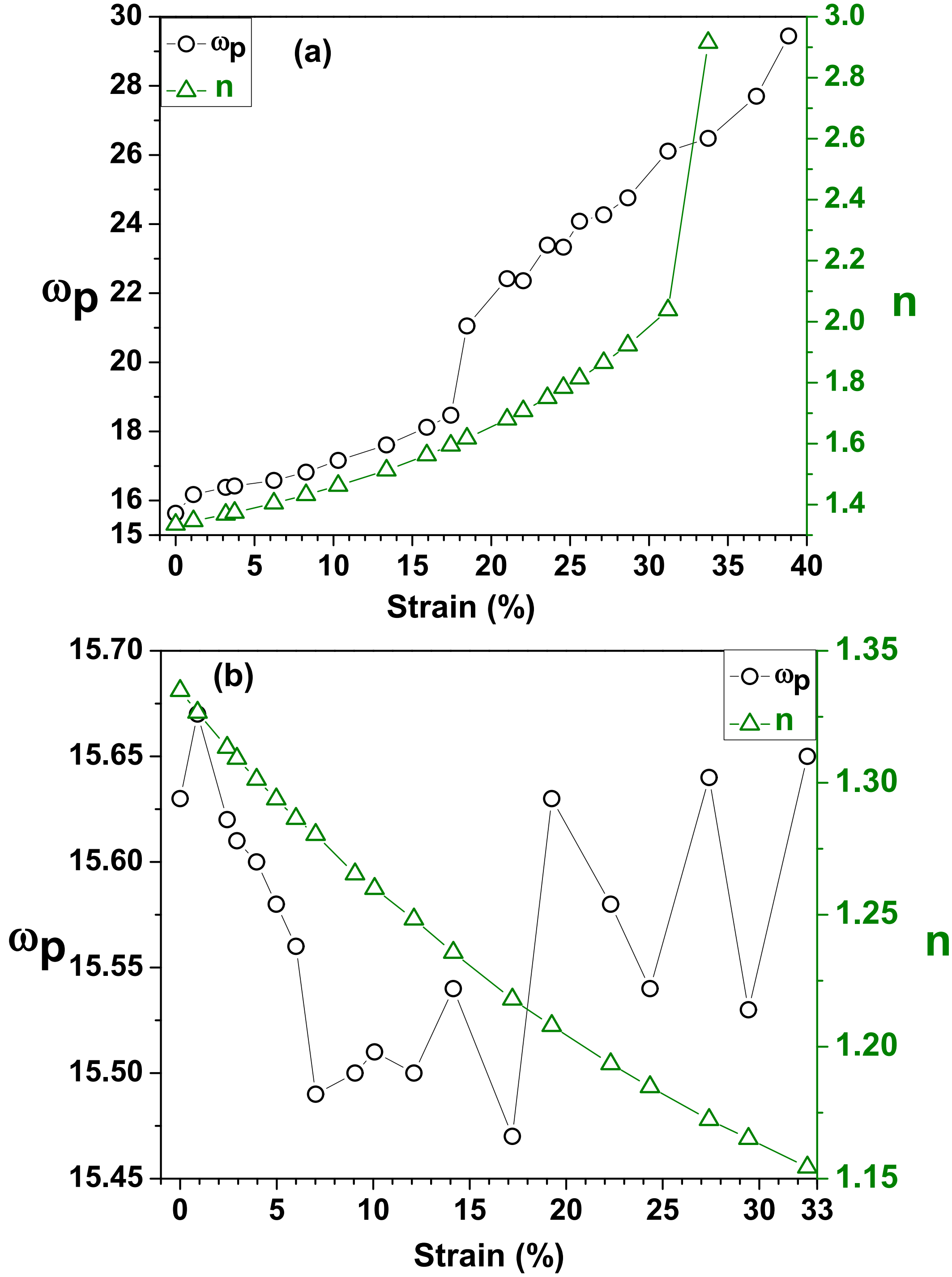


Fig.S8. Radial distribution function (RDF) and Partial RDF for p19, the metallic alloy.

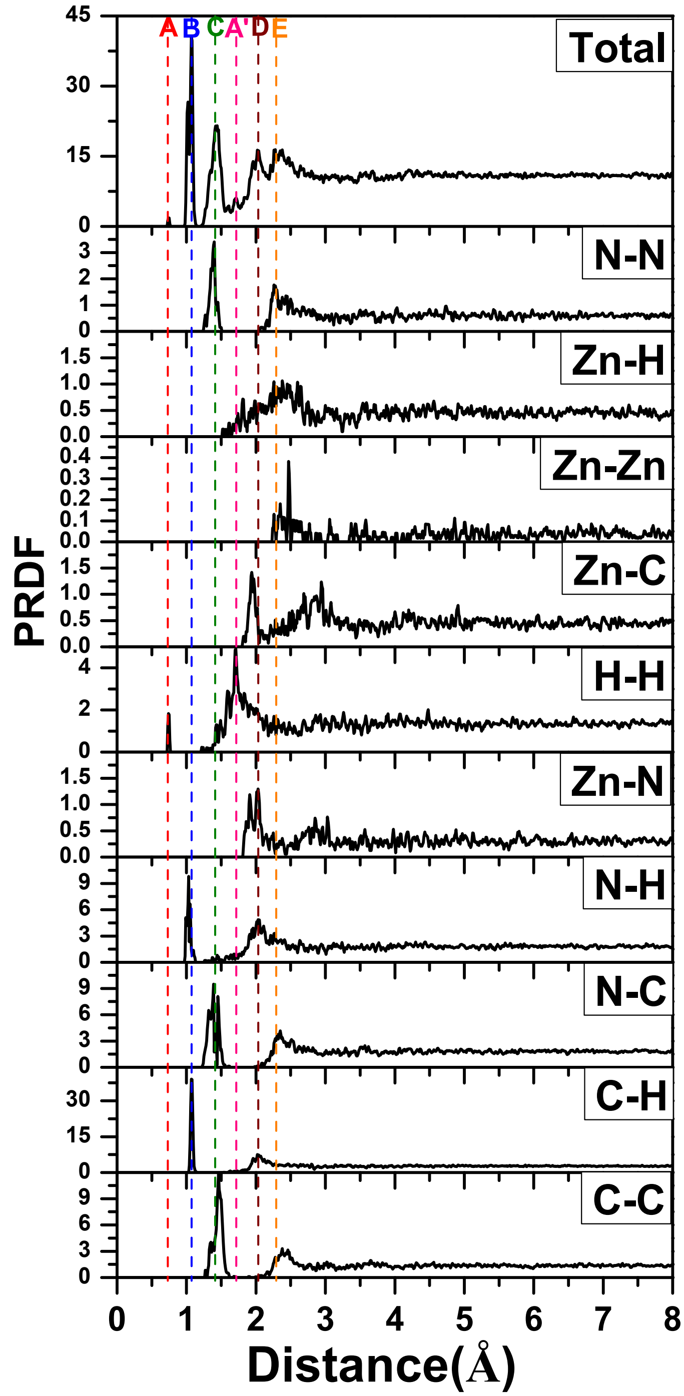
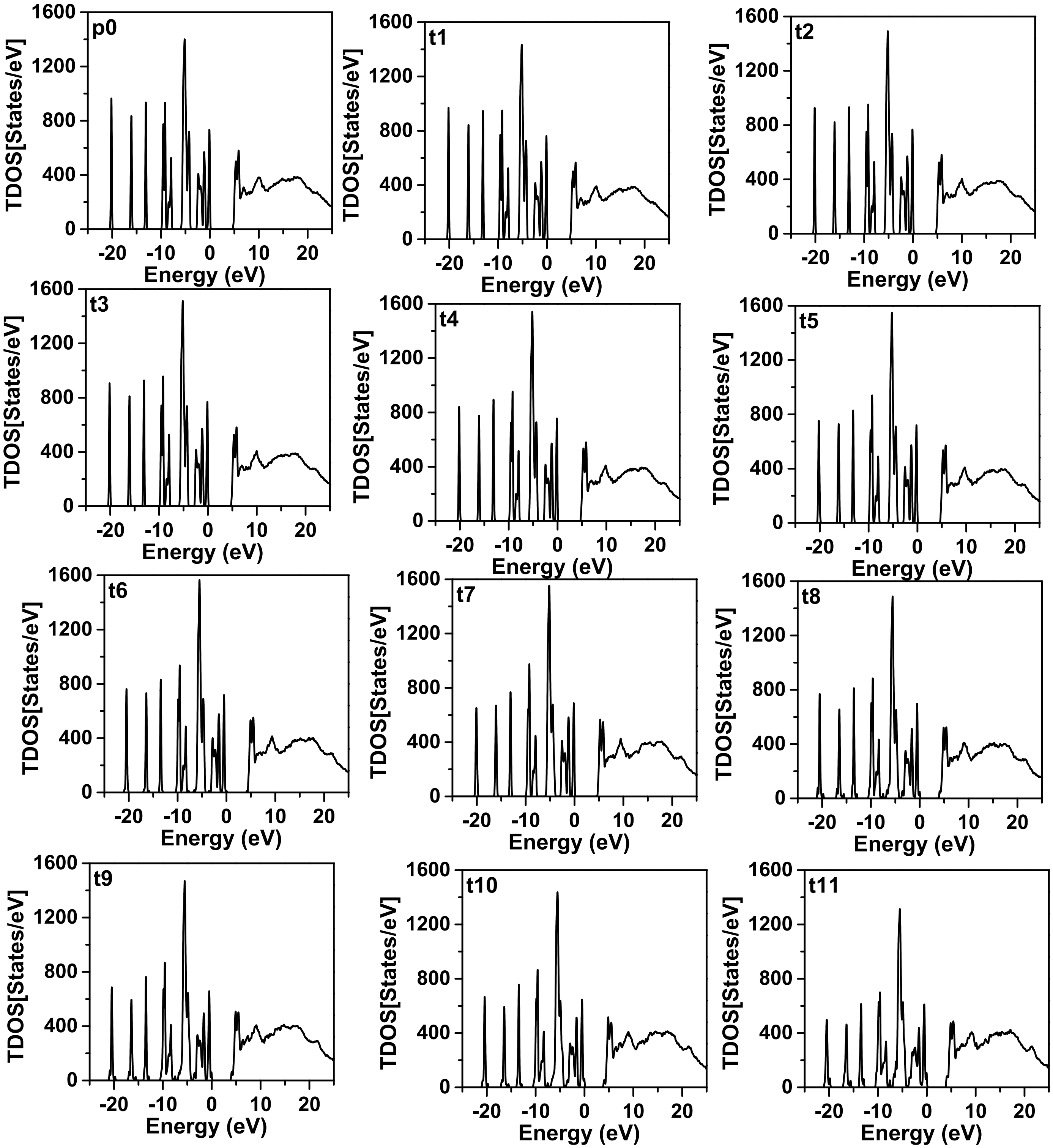


Fig. S9 Total density of states of all data points under expansion.



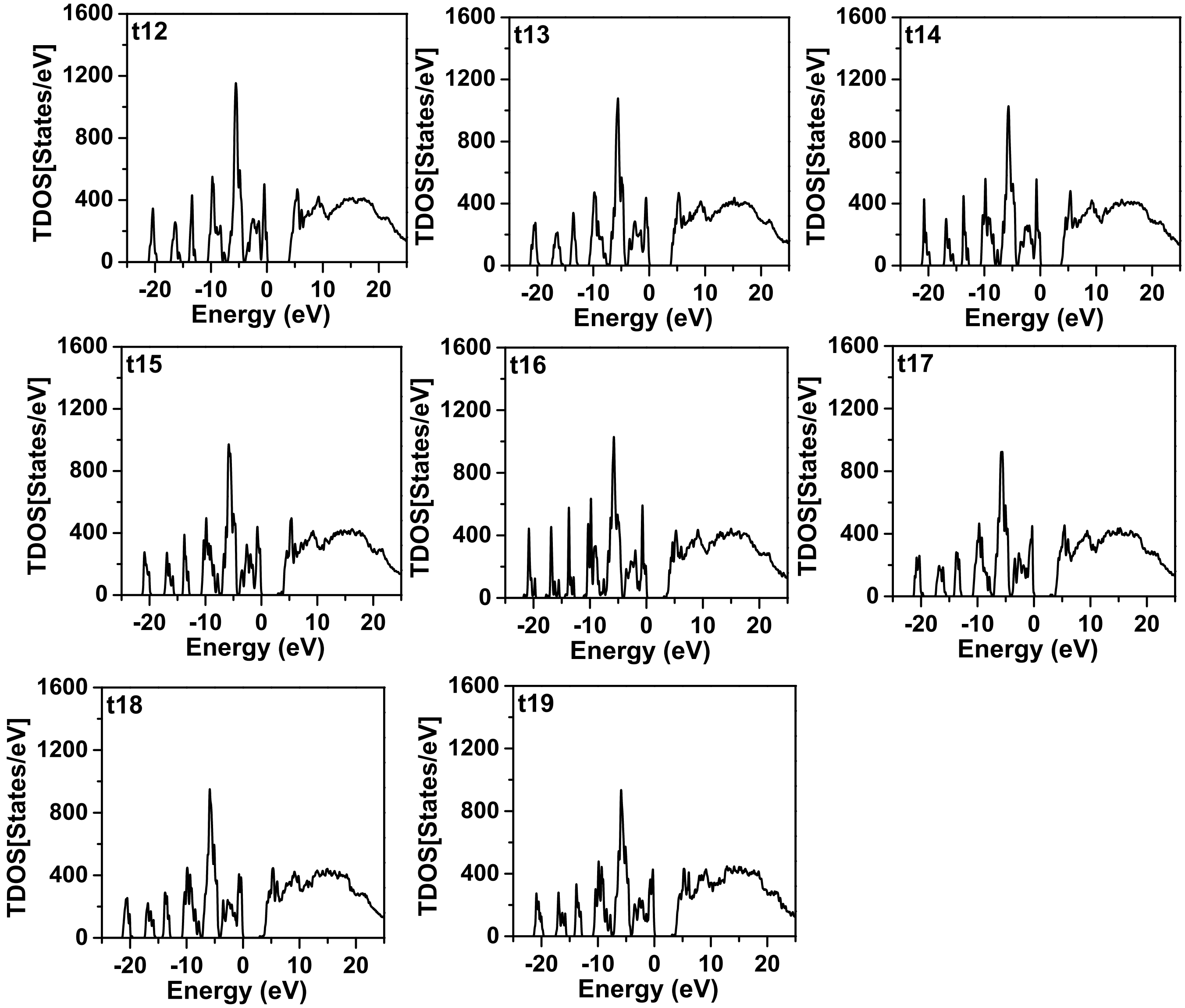

t12
t13
t14
t15
t16
t17
t18
t19
TDOS[States/eV]
Energy (eV)
0
400
800
1200
1600
-20
-10
0
10
20

Fig. S10 Selected partial charge distribution for expansion.

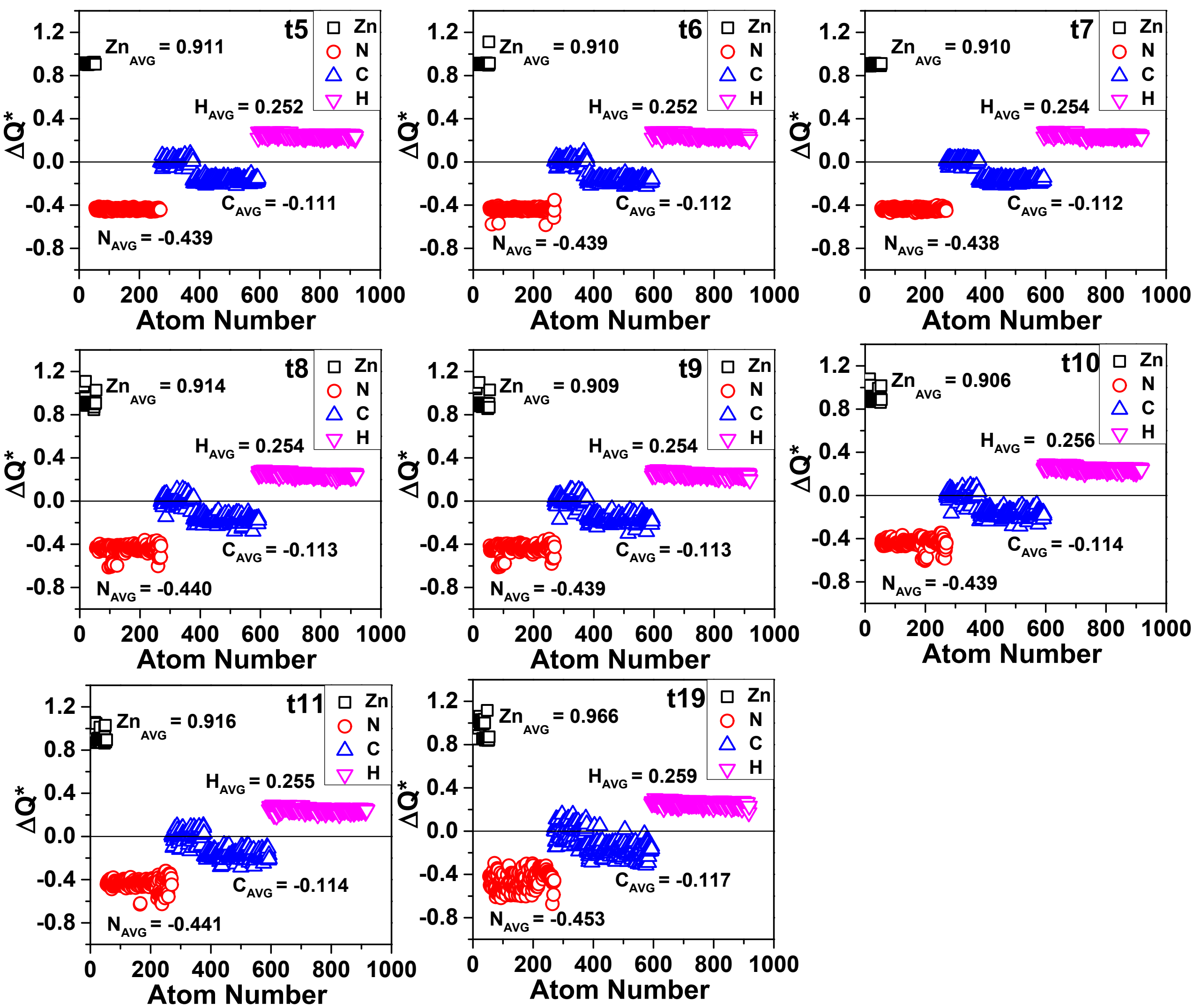
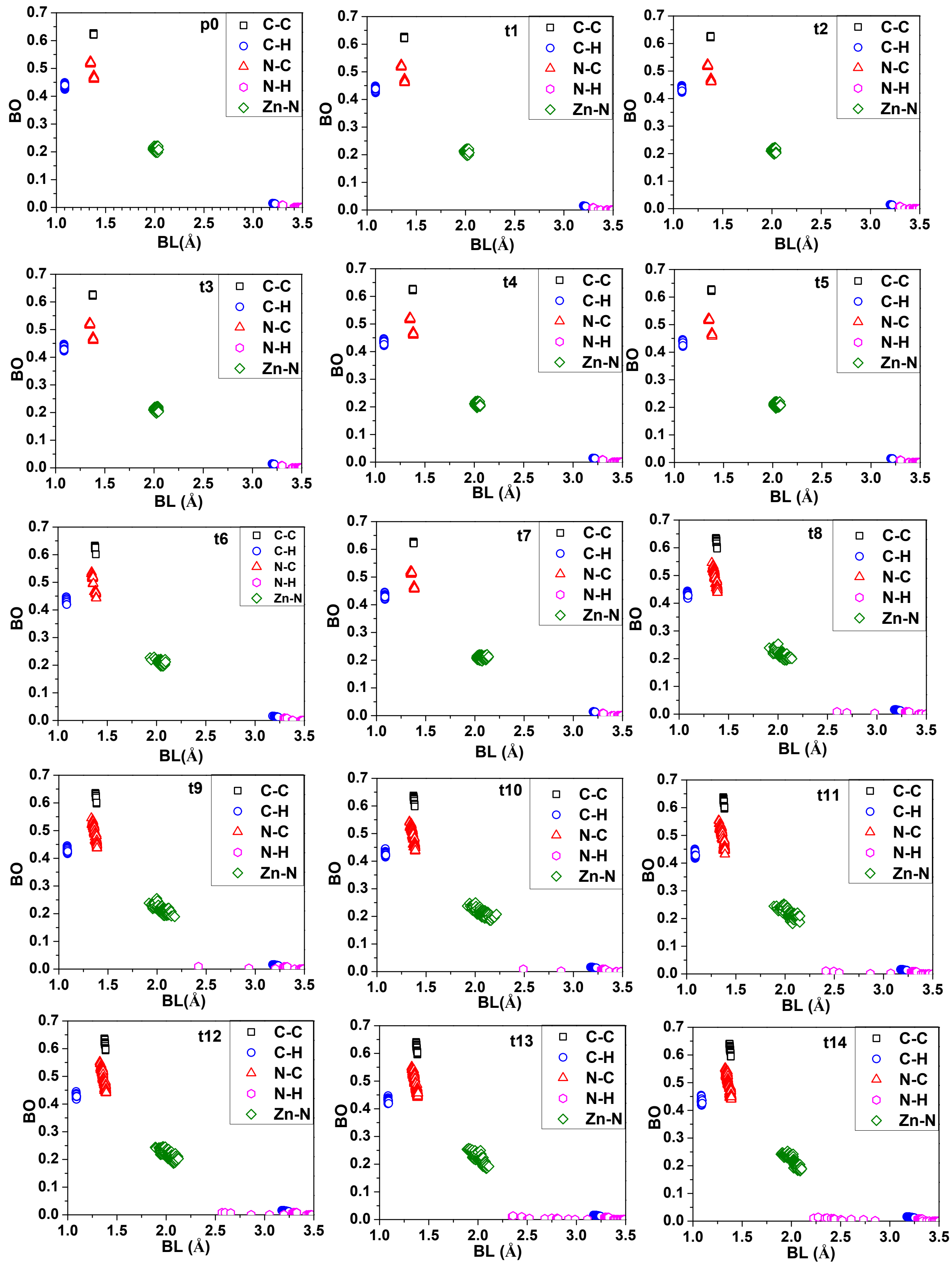


Fig. S11 Bond order (e$^-$) vs. bond length (Å) of all data points under expansion.



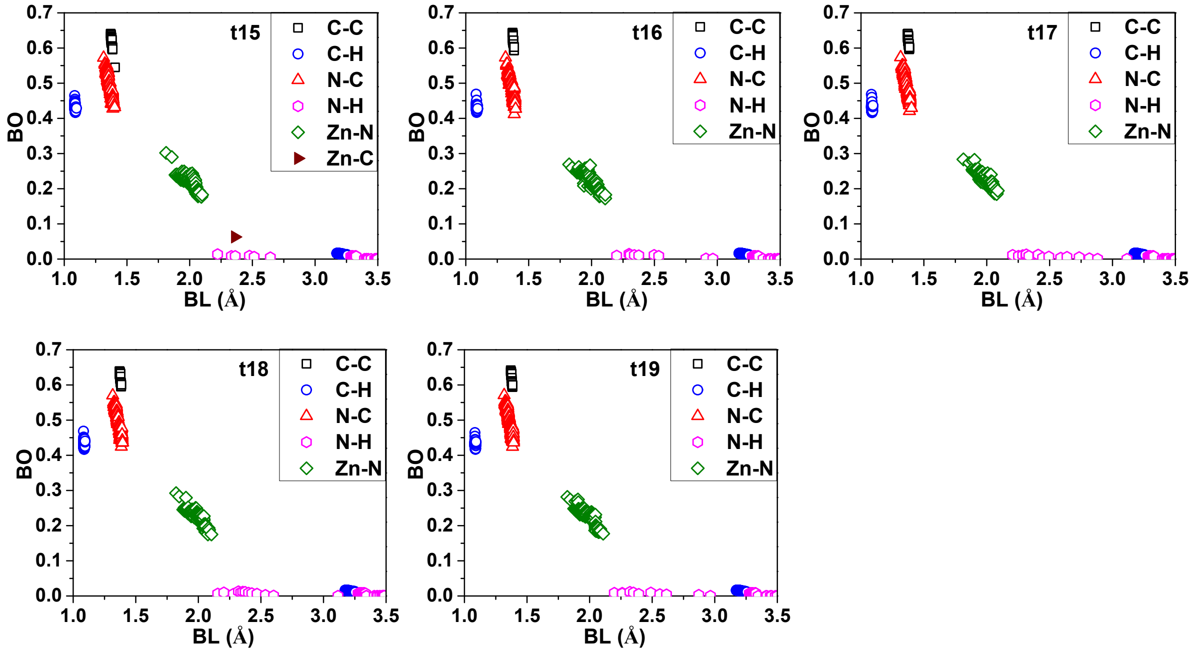
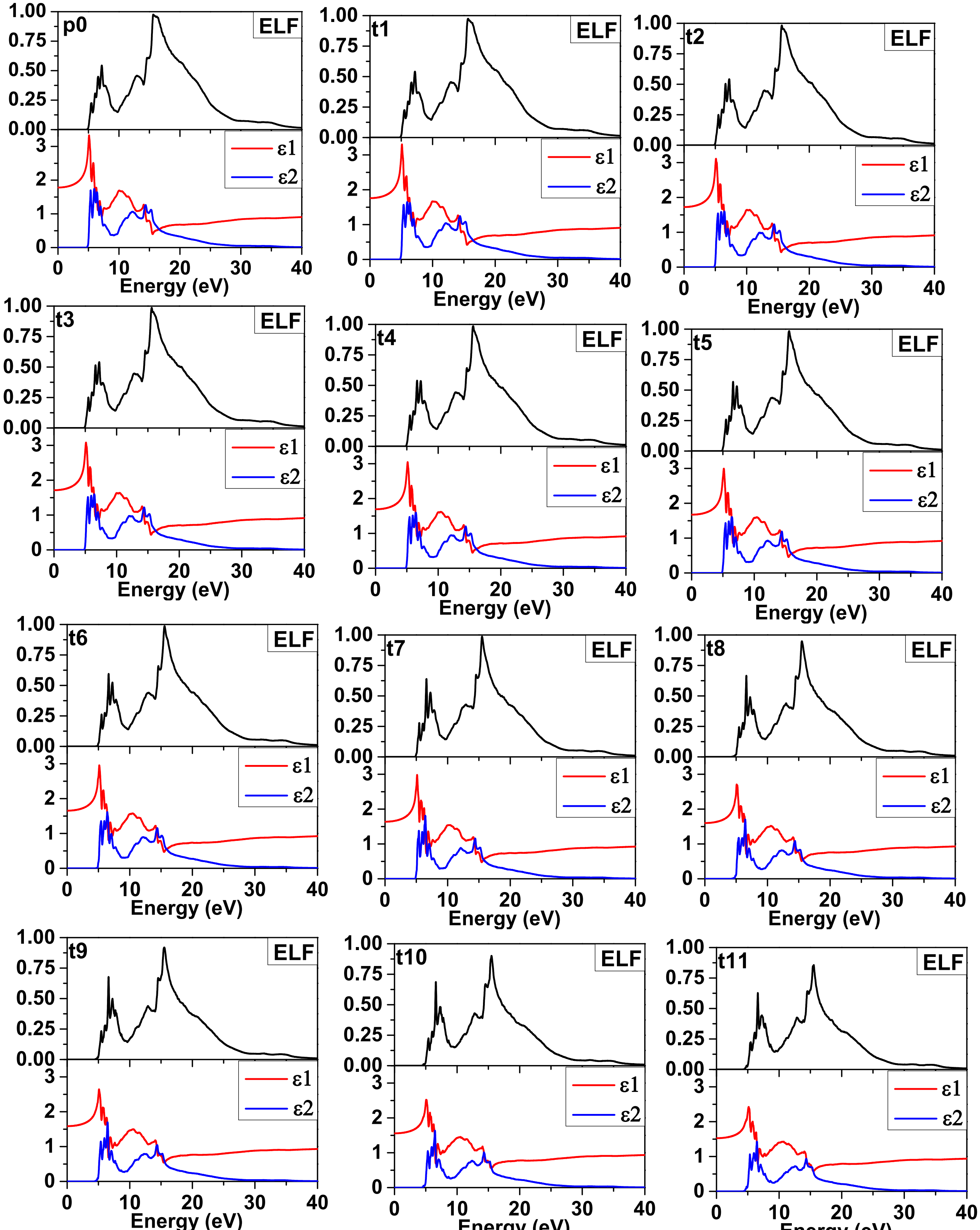
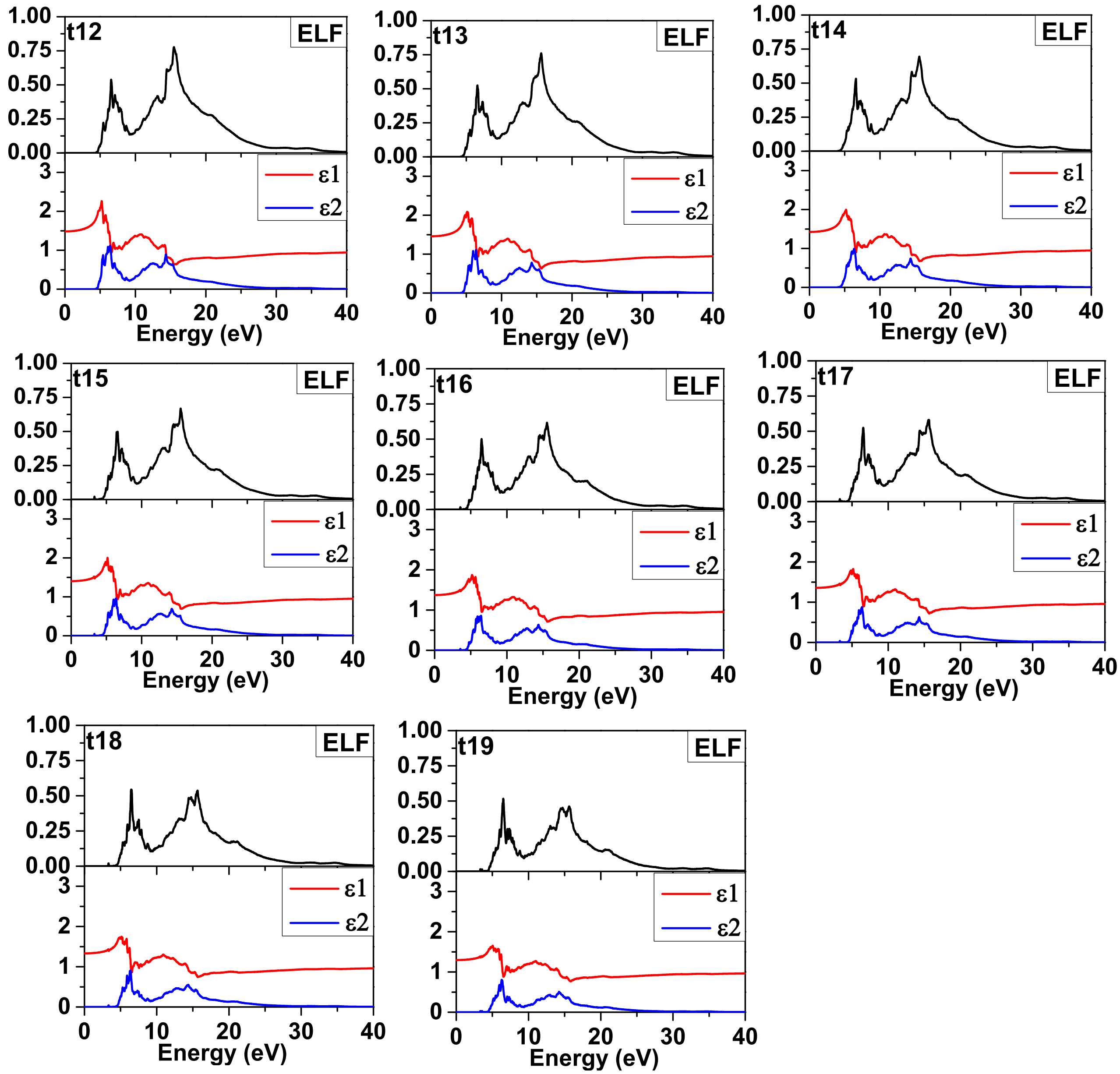

t15
C-C
C-H
N-C
N-H
Zn-N
Zn-C
t16
t17
t18
t19
BO
BL (Å)

Fig. S12 Optical properties of all data points under under expansion**.**




t12
ELF
ε1
ε2
Energy (eV)
t13
ELF
ε1
ε2
Energy (eV)
t14
ELF
ε1
ε2
Energy (eV)
t15
ELF
ε1
ε2
Energy (eV)
t16
ELF
ε1
ε2
Energy (eV)
t17
ELF
ε1
ε2
Energy (eV)
t18
ELF
ε1
ε2
Energy (eV)
t19
ELF
ε1
ε2
Energy (eV)

Supplementary References

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N1_1	N	0.990262	0.401621	0.702010
N1_1	N	0.053266	0.393218	0.761709
N1_1	N	0.001558	0.462653	0.597921
N1_1	N	0.035102	0.530175	0.555197
N1_1	N	0.805116	0.356205	0.996721
N1_1	N	0.864662	0.364359	0.941797
N1_1	N	0.530779	0.329050	0.992914
N1_1	N	0.507114	0.307470	0.912945
N1_1	N	0.565623	0.453421	0.041195
N1_1	N	0.553400	0.542372	0.017821
N1_1	N	0.975592	0.584130	0.460015
N1_1	N	0.950148	0.553802	0.382346
N1_1	N	0.361443	0.979743	0.063274
N1_1	N	0.327852	0.980802	0.137721
N1_1	N	0.417764	0.002250	0.959164
N1_1	N	0.420234	0.053821	0.891790
N1_1	N	0.097736	0.888357	0.071881
N1_1	N	0.086453	0.829361	0.004532
N1_1	N	0.047049	0.992376	0.128065
N1_1	N	0.976604	0.037661	0.098459
N1_1	N	0.042946	0.470679	0.011793
N1_1	N	0.976597	0.419720	0.979035
N1_1	N	0.163591	0.485020	0.045253
N1_1	N	0.205045	0.432868	0.103064
N1_1	N	0.928936	0.802507	0.875726
N1_1	N	0.996853	0.783137	0.927680
N1_1	N	0.934217	0.089683	0.923702
N1_1	N	0.908484	0.056412	0.994338
N1_1	N	0.034385	0.107191	0.851046
N1_1	N	0.110880	0.112228	0.819063
N1_1	N	0.029779	0.681317	0.277463
N1_1	N	0.992071	0.597885	0.282162
N1_1	N	0.084465	0.059367	0.520954
N1_1	N	0.056380	0.977325	0.485383
N1_1	N	0.029691	0.139894	0.600974
N1_1	N	0.947373	0.166708	0.600693
N1_1	N	0.917200	0.221945	0.255974
N1_1	N	0.994965	0.255539	0.278238
N1_1	N	0.006187	0.466616	0.304722
N1_1	N	0.045851	0.381932	0.300432
N1_1	N	0.431960	0.018292	0.285592
N1_1	N	0.360342	0.975936	0.254850
N1_1	N	0.406192	0.987098	0.695565

N1_1	N	0.400218	0.026567	0.772279
C1_1	C	0.505141	0.683726	0.233274
C2_1	C	0.557148	0.752247	0.253002
C2_1	C	0.517827	0.772031	0.221633
C1_1	C	0.641388	0.690870	0.382765
C2_1	C	0.677123	0.609373	0.367006
C2_1	C	0.699576	0.632201	0.410921
C1_1	C	0.686553	0.614987	0.234625
C2_1	C	0.622415	0.578183	0.190319
C2_1	C	0.664659	0.574479	0.162605
C1_1	C	0.543791	0.523992	0.317113
C2_1	C	0.494137	0.596628	0.330118
C2_1	C	0.473411	0.550601	0.349989
C1_1	C	0.877919	0.793621	0.705994
C2_1	C	0.924243	0.862083	0.684612
C2_1	C	0.926994	0.861339	0.735847
C1_1	C	0.788560	0.771322	0.532248
C2_1	C	0.804908	0.701112	0.580065
C2_1	C	0.760650	0.690038	0.551265
C1_1	C	0.320722	0.409202	0.625921
C2_1	C	0.393130	0.375582	0.655703
C2_1	C	0.395951	0.381808	0.605330
C1_1	C	0.364200	0.560016	0.749698
C2_1	C	0.404813	0.515493	0.691733
C2_1	C	0.427282	0.566979	0.702314
C1_1	C	0.221708	0.416791	0.755880
C2_1	C	0.218852	0.490789	0.711174
C2_1	C	0.170251	0.480253	0.724452
C1_1	C	0.389006	0.361176	0.792290
C2_1	C	0.359136	0.427873	0.840545
C2_1	C	0.396384	0.398403	0.867458
C1_1	C	0.734764	0.884570	0.225190
C2_1	C	0.813056	0.860252	0.246259
C2_1	C	0.788370	0.873210	0.288988
C1_1	C	0.778129	0.720447	0.150181
C2_1	C	0.853524	0.737646	0.126545
C2_1	C	0.852109	0.681753	0.137912
C1_1	C	0.371308	0.835455	0.189992
C2_1	C	0.318791	0.776315	0.151081
C2_1	C	0.292362	0.825457	0.162246
C1_1	C	0.349513	0.660934	0.228984
C2_1	C	0.372994	0.601932	0.170589
C2_1	C	0.335989	0.577101	0.195751
C1_1	C	0.694692	0.829049	0.398903
C2_1	C	0.630295	0.847701	0.443917
C2_1	C	0.627326	0.882728	0.404446
C1_1	C	0.624617	0.762127	0.566652
C2_1	C	0.591084	0.694324	0.519200

C2_1	C	0.562452	0.702803	0.560076
C1_1	C	0.620581	0.852042	0.726916
C2_1	C	0.624605	0.890426	0.655697
C2_1	C	0.652917	0.922060	0.691319
C1_1	C	0.484649	0.730980	0.714165
C2_1	C	0.564492	0.709462	0.730984
C2_1	C	0.535803	0.682653	0.763409
C1_1	C	0.479820	0.886403	0.632847
C2_1	C	0.462465	0.821248	0.575313
C2_1	C	0.428469	0.865615	0.568402
C1_1	C	0.640500	0.896737	0.900920
C2_1	C	0.577588	0.896217	0.844359
C2_1	C	0.560722	0.875261	0.887039
C1_1	C	0.774682	0.862655	0.811943
C2_1	C	0.781009	0.940005	0.858064
C2_1	C	0.826709	0.910627	0.862891
C1_1	C	0.494468	0.894710	0.996527
C2_1	C	0.511621	0.842581	0.059701
C2_1	C	0.462087	0.862420	0.061416
C1_1	C	0.566930	0.725803	0.996082
C2_1	C	0.640654	0.723532	0.964186
C2_1	C	0.623505	0.669034	0.965033
C1_1	C	0.529743	0.241835	0.499578
C2_1	C	0.470344	0.272630	0.546709
C2_1	C	0.513722	0.303519	0.558800
C1_1	C	0.482131	0.128470	0.383790
C2_1	C	0.508983	0.073491	0.442448
C2_1	C	0.524935	0.051216	0.397852
C1_1	C	0.329639	0.206656	0.468199
C2_1	C	0.352822	0.154010	0.405213
C2_1	C	0.303429	0.172573	0.394926
C1_1	C	0.787522	0.179477	0.296511
C2_1	C	0.733903	0.246475	0.315524
C2_1	C	0.759114	0.261817	0.275077
C1_1	C	0.685278	0.239004	0.452681
C2_1	C	0.680330	0.152978	0.475886
C2_1	C	0.655308	0.188157	0.508670
C1_1	C	0.821524	0.188498	0.479899
C2_1	C	0.864110	0.136707	0.428195
C2_1	C	0.893957	0.144594	0.471965
C1_1	C	0.641135	0.343737	0.631484
C2_1	C	0.697481	0.380806	0.587996
C2_1	C	0.707227	0.397800	0.637234
C1_1	C	0.575559	0.365520	0.433953
C2_1	C	0.637558	0.419599	0.461934
C2_1	C	0.609599	0.446501	0.424614
C1_1	C	0.919055	0.313462	0.605462
C2_1	C	0.854506	0.371995	0.601759

C2_1	C	0.837141	0.318561	0.588840
C1_1	C	0.894421	0.501399	0.711001
C2_1	C	0.869385	0.528548	0.637482
C2_1	C	0.841085	0.557518	0.672112
C1_1	C	0.864684	0.149603	0.814831
C2_1	C	0.867408	0.092775	0.749560
C2_1	C	0.914751	0.092493	0.774877
C1_1	C	0.811337	0.182359	0.659678
C2_1	C	0.760305	0.113422	0.638047
C2_1	C	0.789845	0.122677	0.598837
C1_1	C	0.721719	0.267786	0.743268
C2_1	C	0.737922	0.250753	0.821297
C2_1	C	0.716484	0.304085	0.818300
C1_1	C	0.665284	0.349459	0.050466
C2_1	C	0.696746	0.331426	0.124645
C2_1	C	0.644318	0.331153	0.124538
C1_1	C	0.825886	0.295062	0.132893
C2_1	C	0.845646	0.380238	0.159092
C2_1	C	0.859526	0.344072	0.196365
C1_1	C	0.768390	0.488143	0.112916
C2_1	C	0.789173	0.499326	0.037436
C2_1	C	0.790941	0.550995	0.063100
C1_1	C	0.494170	0.320985	0.132944
C2_1	C	0.475698	0.409978	0.126190
C2_1	C	0.445185	0.388624	0.160214
C1_1	C	0.461975	0.356831	0.290643
C2_1	C	0.435920	0.327865	0.359772
C2_1	C	0.415566	0.293701	0.320951
C1_1	C	0.412648	0.440129	0.445995
C2_1	C	0.482213	0.474615	0.482338
C2_1	C	0.445029	0.476959	0.516128
C1_1	C	0.136735	0.628313	0.504118
C2_1	C	0.083401	0.678230	0.458625
C2_1	C	0.132043	0.696117	0.452401
C1_1	C	0.325419	0.869620	0.926823
C2_1	C	0.281421	0.934110	0.965700
C2_1	C	0.249346	0.906427	0.930543
C1_1	C	0.071841	0.826458	0.203624
C2_1	C	0.008738	0.886347	0.208485
C2_1	C	0.004726	0.846964	0.243987
C1_1	C	0.201865	0.945448	0.169066
C2_1	C	0.157442	0.945402	0.234263
C2_1	C	0.207986	0.952674	0.249932
C1_1	C	0.091484	0.641944	0.981071
C2_1	C	0.053771	0.622807	0.047432
C2_1	C	0.043330	0.678304	0.037079
C1_1	C	0.109162	0.456578	0.901961
C2_1	C	0.155761	0.531177	0.904499

C2_1	C	0.159053	0.503633	0.858621
C1_1	C	0.869598	0.566675	0.241073
C2_1	C	0.804557	0.515221	0.253077
C2_1	C	0.845737	0.496653	0.282667
C1_1	C	0.225726	0.764831	0.564932
C2_1	C	0.306548	0.757540	0.552944
C2_1	C	0.299826	0.798027	0.590374
C1_1	C	0.284820	0.555623	0.510427
C2_1	C	0.281151	0.601745	0.581565
C2_1	C	0.303885	0.549852	0.589674
C1_1	C	0.249958	0.643105	0.382603
C2_1	C	0.325862	0.651236	0.418965
C2_1	C	0.330440	0.632299	0.370265
C1_1	C	0.850775	0.678554	0.792537
C2_1	C	0.805195	0.715720	0.850295
C2_1	C	0.795023	0.658994	0.844948
C1_1	C	0.948780	0.261780	0.888555
C2_1	C	0.023770	0.237206	0.919665
C2_1	C	0.017948	0.294722	0.926846
C1_1	C	0.162201	0.784797	0.907757
C2_1	C	0.115883	0.726452	0.860490
C2_1	C	0.158736	0.738403	0.836270
C1_1	C	0.879006	0.124534	0.145881
C2_1	C	0.809923	0.100966	0.101650
C2_1	C	0.797160	0.140001	0.138470
C1_1	C	0.043413	0.815964	0.389396
C2_1	C	0.121773	0.824220	0.369933
C2_1	C	0.113871	0.859851	0.410588
C1_1	C	0.160194	0.673534	0.273785
C2_1	C	0.180449	0.758766	0.257982
C2_1	C	0.221714	0.723541	0.250196
C1_1	C	0.134546	0.133813	0.680682
C2_1	C	0.183329	0.069964	0.646988
C2_1	C	0.201239	0.080572	0.695749
C1_1	C	0.160658	0.180957	0.505316
C2_1	C	0.135390	0.238979	0.563676
C2_1	C	0.167252	0.267251	0.535115
C1_1	C	0.145619	0.277962	0.357891
C2_1	C	0.157073	0.187131	0.355046
C2_1	C	0.117655	0.200324	0.321014
C1_1	C	0.283009	0.352088	0.464423
C2_1	C	0.202901	0.375919	0.456354
C2_1	C	0.229999	0.422091	0.475281
C1_1	C	0.878077	0.466667	0.855652
C2_1	C	0.934522	0.521377	0.828918
C2_1	C	0.959684	0.478589	0.853715
C1_1	C	0.751173	0.464477	0.768813
C2_1	C	0.713587	0.542684	0.791934

C2_1	C	0.676873	0.502653	0.780376
C1_1	C	0.139647	0.274441	0.788379
C2_1	C	0.182558	0.310618	0.853502
C2_1	C	0.194326	0.253899	0.849112
C1_1	C	0.479165	0.636709	0.887625
C2_1	C	0.471486	0.557567	0.844306
C2_1	C	0.490094	0.546190	0.891899
C1_1	C	0.344419	0.744453	0.811019
C2_1	C	0.348561	0.670238	0.855419
C2_1	C	0.307543	0.703031	0.868971
C1_1	C	0.468102	0.174716	0.248046
C2_1	C	0.481013	0.113942	0.187322
C2_1	C	0.460344	0.162499	0.167580
C1_1	C	0.124972	0.864734	0.556003
C2_1	C	0.096243	0.876432	0.629612
C2_1	C	0.055758	0.879337	0.594534
C1_1	C	0.235368	0.833611	0.739211
C2_1	C	0.213496	0.922180	0.735537
C2_1	C	0.225117	0.910532	0.784648
C1_1	C	0.297487	0.945260	0.630385
C2_1	C	0.252148	0.950637	0.560554
C2_1	C	0.299219	0.973534	0.555153
C1_1	C	0.318889	0.332697	0.190515
C2_1	C	0.319363	0.251840	0.149424
C2_1	C	0.273923	0.279438	0.137295
C1_1	C	0.283387	0.119327	0.804183
C2_1	C	0.245472	0.110176	0.872474
C2_1	C	0.297000	0.100829	0.882139
C1_1	C	0.138872	0.328772	0.216606
C2_1	C	0.074530	0.307543	0.165200
C2_1	C	0.111844	0.330506	0.138967
C1_1	C	0.578346	0.345793	0.792703
C2_1	C	0.555949	0.414107	0.744567
C2_1	C	0.514408	0.400084	0.769821
C1_1	C	0.431993	0.204120	0.826052
C2_1	C	0.481587	0.146577	0.785784
C2_1	C	0.502457	0.199528	0.788105
C1_1	C	0.227520	0.500065	0.220206
C2_1	C	0.242496	0.433734	0.272241
C2_1	C	0.249293	0.485073	0.297700
C1_1	C	0.951962	0.690791	0.556025
C2_1	C	0.980177	0.717112	0.630913
C2_1	C	0.011713	0.674663	0.613368
C1_1	C	0.952641	0.837999	0.523502
C2_1	C	0.891655	0.898918	0.535949
C2_1	C	0.925528	0.922189	0.506011
C1_1	C	0.692493	0.837895	0.062448
C2_1	C	0.706384	0.923082	0.092515

C2_1	C	0.665547	0.924731	0.057790
C1_1	C	0.851886	0.941705	0.106770
C2_1	C	0.863355	0.868600	0.057083
C2_1	C	0.886627	0.914053	0.038644
C1_1	C	0.474539	0.664828	0.079715
C2_1	C	0.401342	0.700112	0.053410
C2_1	C	0.423090	0.672424	0.013773
C1_1	C	0.721505	0.040527	0.777290
C2_1	C	0.643640	0.057384	0.796902
C2_1	C	0.663786	0.106883	0.782700
C1_1	C	0.720591	0.040407	0.349574
C2_1	C	0.745083	0.982777	0.407010
C2_1	C	0.761312	0.036037	0.422151
C1_1	C	0.597962	0.996955	0.299073
C2_1	C	0.592794	0.925016	0.246342
C2_1	C	0.549860	0.958598	0.238686
C1_1	C	0.413394	0.075472	0.553133
C2_1	C	0.482280	0.118967	0.580630
C2_1	C	0.474958	0.075193	0.611056
C1_1	C	0.037511	0.417224	0.718859
C2_1	C	0.974682	0.365136	0.736305
C2_1	C	0.013364	0.359948	0.773015
C1_1	C	0.000980	0.517740	0.588074
C2_1	C	0.038659	0.438057	0.569540
C2_1	C	0.059174	0.479558	0.543193
C1_1	C	0.852282	0.373745	0.989119
C2_1	C	0.785928	0.334060	0.951181
C2_1	C	0.822628	0.339005	0.917320
C1_1	C	0.523524	0.347995	0.946596
C2_1	C	0.518293	0.272744	0.988621
C2_1	C	0.503698	0.259456	0.939502
C1_1	C	0.532033	0.491916	0.022600
C2_1	C	0.611415	0.481185	0.048813
C2_1	C	0.603913	0.535745	0.034356
C1_1	C	0.989994	0.565037	0.415137
C2_1	C	0.922873	0.584729	0.455767
C2_1	C	0.907251	0.566362	0.407939
C1_1	C	0.345795	0.948940	0.099872
C2_1	C	0.352858	0.035272	0.078534
C2_1	C	0.332122	0.035920	0.124337
C1_1	C	0.396322	0.012992	0.913774
C2_1	C	0.458298	0.038567	0.966768
C2_1	C	0.459801	0.070271	0.925270
C1_1	C	0.089997	0.834684	0.054693
C2_1	C	0.099280	0.919395	0.029855
C2_1	C	0.092309	0.883245	0.988590
C1_1	C	0.999252	0.987521	0.107325
C2_1	C	0.055839	0.049565	0.132826

C2_1	C	0.012485	0.077460	0.114505
C1_1	C	0.005502	0.465451	0.975270
C2_1	C	0.037173	0.425551	0.041475
C2_1	C	0.996515	0.394338	0.021422
C1_1	C	0.163241	0.464557	0.091076
C2_1	C	0.208764	0.465190	0.026759
C2_1	C	0.234224	0.433293	0.062250
C1_1	C	0.978213	0.785120	0.879889
C2_1	C	0.915227	0.812106	0.924145
C2_1	C	0.956884	0.800346	0.955910
C1_1	C	0.941598	0.089562	0.973687
C2_1	C	0.893729	0.054123	0.911585
C2_1	C	0.877935	0.033764	0.954962
C1_1	C	0.069294	0.140844	0.833625
C2_1	C	0.055062	0.053293	0.847242
C2_1	C	0.102014	0.056381	0.827507
C1_1	C	0.008766	0.645215	0.307115
C2_1	C	0.026171	0.655339	0.230340
C2_1	C	0.003155	0.604083	0.233301
C1_1	C	0.074499	0.004922	0.527632
C2_1	C	0.071689	0.067294	0.471054
C2_1	C	0.054551	0.016855	0.449243
C1_1	C	0.991529	0.169627	0.578197
C2_1	C	0.008495	0.116264	0.640604
C2_1	C	0.957957	0.132868	0.640502
C1_1	C	0.956839	0.251566	0.242380
C2_1	C	0.930889	0.205946	0.303734
C2_1	C	0.978684	0.226504	0.317432
C1_1	C	0.000760	0.410186	0.300022
C2_1	C	0.058275	0.474966	0.308558
C2_1	C	0.082536	0.423119	0.305895
C1_1	C	0.399250	0.009375	0.245594
C2_1	C	0.412865	0.988709	0.323030
C2_1	C	0.368837	0.962626	0.304131
C1_1	C	0.400541	0.035261	0.723239
C2_1	C	0.409536	0.944715	0.729160
C2_1	C	0.405949	0.969014	0.776307
H1_1	H	0.487710	0.642478	0.231419
H2_1	H	0.589923	0.774201	0.270652
H2_1	H	0.511067	0.813934	0.207805
H1_1	H	0.616667	0.727956	0.379618
H2_1	H	0.684999	0.569638	0.347123
H2_1	H	0.730149	0.615595	0.435443
H1_1	H	0.709163	0.635240	0.265431
H2_1	H	0.583714	0.564298	0.180811
H2_1	H	0.668754	0.556671	0.125263
H1_1	H	0.575565	0.497826	0.305237
H2_1	H	0.480602	0.640100	0.329539

H2_1	H	0.439067	0.547250	0.369887
H1_1	H	0.852386	0.757986	0.703827
H2_1	H	0.941936	0.890149	0.660392
H2_1	H	0.947304	0.888825	0.763446
H1_1	H	0.791781	0.811162	0.514501
H2_1	H	0.825364	0.675890	0.607741
H2_1	H	0.735521	0.654195	0.550609
H1_1	H	0.281806	0.425775	0.623603
H2_1	H	0.422067	0.360635	0.682852
H2_1	H	0.427236	0.373391	0.581551
H1_1	H	0.337031	0.570024	0.777681
H2_1	H	0.414404	0.481697	0.665230
H2_1	H	0.459659	0.585552	0.686507
H1_1	H	0.236199	0.380685	0.776159
H2_1	H	0.232393	0.523680	0.688887
H2_1	H	0.134846	0.503184	0.715886
H1_1	H	0.394691	0.333406	0.759828
H2_1	H	0.335680	0.463713	0.851980
H2_1	H	0.410502	0.404231	0.906122
H1_1	H	0.700144	0.894257	0.202642
H2_1	H	0.852106	0.846140	0.241734
H2_1	H	0.802784	0.873338	0.327713
H1_1	H	0.738806	0.726011	0.159948
H2_1	H	0.884616	0.761755	0.114160
H2_1	H	0.881573	0.649147	0.136153
H1_1	H	0.405795	0.853618	0.208095
H2_1	H	0.305396	0.737154	0.132728
H2_1	H	0.252362	0.836277	0.154609
H1_1	H	0.346988	0.698710	0.253164
H2_1	H	0.393386	0.585897	0.138974
H2_1	H	0.319284	0.535669	0.189947
H1_1	H	0.729002	0.809301	0.385118
H2_1	H	0.604894	0.844030	0.473762
H2_1	H	0.599079	0.914962	0.394559
H1_1	H	0.650191	0.795274	0.581250
H2_1	H	0.586432	0.664223	0.487682
H2_1	H	0.528896	0.680987	0.570033
H1_1	H	0.610562	0.823717	0.755157
H2_1	H	0.617124	0.896793	0.616206
H2_1	H	0.674221	0.960269	0.687935
H1_1	H	0.450209	0.749176	0.696403
H2_1	H	0.605464	0.708571	0.727661
H2_1	H	0.547449	0.654952	0.793165
H1_1	H	0.498214	0.909174	0.664866
H2_1	H	0.466258	0.781719	0.553806
H2_1	H	0.397208	0.870562	0.540425
H1_1	H	0.678246	0.902261	0.919375
H2_1	H	0.557247	0.902374	0.808571

H2_1	H	0.523521	0.859419	0.894049
H1_1	H	0.759348	0.829693	0.786153
H2_1	H	0.769729	0.980375	0.874960
H2_1	H	0.861722	0.921370	0.884662
H1_1	H	0.498599	0.917854	0.963223
H2_1	H	0.533571	0.815574	0.084905
H2_1	H	0.434091	0.855034	0.088178
H1_1	H	0.532309	0.741337	0.012361
H2_1	H	0.675559	0.739106	0.950697
H2_1	H	0.641081	0.629615	0.952372
H1_1	H	0.549776	0.216811	0.471971
H2_1	H	0.433457	0.275229	0.562662
H2_1	H	0.520303	0.338133	0.586141
H1_1	H	0.463528	0.163472	0.364854
H2_1	H	0.514913	0.058107	0.479752
H2_1	H	0.546866	0.012989	0.390055
H1_1	H	0.330146	0.228965	0.504402
H2_1	H	0.376831	0.126409	0.383139
H2_1	H	0.277911	0.164636	0.362076
H1_1	H	0.809052	0.139910	0.297110
H2_1	H	0.704290	0.268788	0.335180
H2_1	H	0.755492	0.299849	0.254172
H1_1	H	0.694271	0.275281	0.431904
H2_1	H	0.685932	0.107521	0.475114
H2_1	H	0.635535	0.178281	0.541228
H1_1	H	0.790849	0.213161	0.495851
H2_1	H	0.872115	0.112525	0.394293
H2_1	H	0.932127	0.128839	0.482131
H1_1	H	0.608819	0.319754	0.641507
H2_1	H	0.717569	0.390448	0.555566
H2_1	H	0.736733	0.425023	0.654510
H1_1	H	0.549583	0.330290	0.429661
H2_1	H	0.670939	0.433735	0.484665
H2_1	H	0.614759	0.487648	0.409820
H1_1	H	0.957545	0.296408	0.611416
H2_1	H	0.833819	0.411908	0.604734
H2_1	H	0.798625	0.304388	0.578825
H1_1	H	0.915186	0.479263	0.740574
H2_1	H	0.867794	0.530888	0.597226
H2_1	H	0.810594	0.588635	0.666790
H1_1	H	0.850499	0.179135	0.842952
H2_1	H	0.854184	0.070227	0.715248
H2_1	H	0.949464	0.069396	0.766514
H1_1	H	0.830837	0.216063	0.681557
H2_1	H	0.730574	0.082884	0.641168
H2_1	H	0.789869	0.101744	0.562135
H1_1	H	0.718919	0.262666	0.702875
H2_1	H	0.750545	0.227560	0.853805

H2_1	H	0.708237	0.335221	0.847641
H1_1	H	0.662360	0.359730	0.011463
H2_1	H	0.725495	0.324090	0.154559
H2_1	H	0.619872	0.323901	0.154489
H1_1	H	0.811598	0.259573	0.109392
H2_1	H	0.849430	0.425635	0.158480
H2_1	H	0.877357	0.352887	0.233347
H1_1	H	0.757075	0.468519	0.146046
H2_1	H	0.797207	0.488116	0.999172
H2_1	H	0.800695	0.592125	0.050849
H1_1	H	0.512088	0.279652	0.127743
H2_1	H	0.477830	0.452487	0.113352
H2_1	H	0.416001	0.409618	0.181407
H1_1	H	0.481008	0.381091	0.264317
H2_1	H	0.431658	0.326432	0.399509
H2_1	H	0.389941	0.258393	0.321527
H1_1	H	0.385612	0.421576	0.417892
H2_1	H	0.521770	0.487435	0.486741
H2_1	H	0.446667	0.492756	0.554676
H1_1	H	0.152237	0.597485	0.529874
H2_1	H	0.047018	0.693305	0.442444
H2_1	H	0.144656	0.729295	0.429889
H1_1	H	0.356922	0.842538	0.915754
H2_1	H	0.273471	0.968402	0.992308
H2_1	H	0.208819	0.912941	0.921580
H1_1	H	0.106527	0.805463	0.192083
H2_1	H	0.984575	0.922653	0.199805
H2_1	H	0.976371	0.843508	0.271196
H1_1	H	0.212075	0.943640	0.130558
H2_1	H	0.124064	0.943133	0.255757
H2_1	H	0.225768	0.958056	0.287356
H1_1	H	0.113694	0.637518	0.948463
H2_1	H	0.041203	0.598063	0.077089
H2_1	H	0.020229	0.709572	0.056432
H1_1	H	0.084064	0.424189	0.912962
H2_1	H	0.174112	0.569547	0.919333
H2_1	H	0.180066	0.514377	0.827110
H1_1	H	0.893070	0.599109	0.227527
H2_1	H	0.765639	0.500258	0.249150
H2_1	H	0.848395	0.462893	0.308606
H1_1	H	0.184860	0.757901	0.561277
H2_1	H	0.341343	0.742189	0.536958
H2_1	H	0.327794	0.824328	0.611325
H1_1	H	0.281585	0.545518	0.470577
H2_1	H	0.273465	0.636610	0.607695
H2_1	H	0.319447	0.532364	0.624081
H1_1	H	0.208667	0.644124	0.376330
H2_1	H	0.355217	0.659787	0.448493

H2_1	H	0.364275	0.622376	0.350265
H1_1	H	0.877775	0.673589	0.763687
H2_1	H	0.789961	0.748067	0.875297
H2_1	H	0.769866	0.633792	0.864972
H1_1	H	0.910664	0.259598	0.870396
H2_1	H	0.055990	0.209877	0.929896
H2_1	H	0.043882	0.325267	0.945293
H1_1	H	0.175346	0.812245	0.939237
H2_1	H	0.084358	0.698932	0.848773
H2_1	H	0.170281	0.723210	0.799993
H1_1	H	0.918756	0.126304	0.159783
H2_1	H	0.785909	0.079588	0.072572
H2_1	H	0.760217	0.157971	0.146876
H1_1	H	0.004053	0.802564	0.388950
H2_1	H	0.155822	0.816684	0.349692
H2_1	H	0.139822	0.888879	0.431149
H1_1	H	0.138339	0.637808	0.283740
H2_1	H	0.176453	0.803991	0.253977
H2_1	H	0.258827	0.733337	0.237685
H1_1	H	0.103744	0.164391	0.685474
H2_1	H	0.197915	0.040953	0.618742
H2_1	H	0.233566	0.061972	0.716615
H1_1	H	0.165782	0.142701	0.482290
H2_1	H	0.115824	0.253752	0.596211
H2_1	H	0.179608	0.310714	0.538394
H1_1	H	0.149951	0.322434	0.368435
H2_1	H	0.173476	0.146267	0.364176
H2_1	H	0.094467	0.172976	0.295633
H1_1	H	0.318118	0.327157	0.463939
H2_1	H	0.162134	0.371569	0.447956
H2_1	H	0.216802	0.464303	0.485847
H1_1	H	0.841694	0.449279	0.863657
H2_1	H	0.949788	0.556373	0.810390
H2_1	H	0.000337	0.470148	0.859517
H1_1	H	0.780692	0.433772	0.759525
H2_1	H	0.709444	0.586602	0.804318
H2_1	H	0.635707	0.505791	0.781793
H1_1	H	0.113929	0.270680	0.755131
H2_1	H	0.196263	0.342504	0.881142
H2_1	H	0.220193	0.228344	0.872140
H1_1	H	0.478560	0.681535	0.897916
H2_1	H	0.462698	0.529049	0.812343
H2_1	H	0.500568	0.506168	0.907951
H1_1	H	0.352872	0.775047	0.784052
H2_1	H	0.363058	0.630448	0.869350
H2_1	H	0.279995	0.696363	0.896348
H1_1	H	0.467148	0.194627	0.285106
H2_1	H	0.492809	0.074804	0.168601

H2_1	H	0.450975	0.172123	0.128996
H1_1	H	0.150937	0.857519	0.526482
H2_1	H	0.096997	0.880057	0.669985
H2_1	H	0.015398	0.886010	0.599458
H1_1	H	0.243925	0.790031	0.728068
H2_1	H	0.201219	0.961456	0.719016
H2_1	H	0.225062	0.938175	0.817934
H1_1	H	0.309067	0.936400	0.668775
H2_1	H	0.219503	0.946063	0.533856
H2_1	H	0.313861	0.991929	0.522918
H1_1	H	0.330333	0.367912	0.215779
H2_1	H	0.333303	0.210706	0.136550
H2_1	H	0.241686	0.266054	0.112553
H1_1	H	0.289830	0.127099	0.765674
H2_1	H	0.214391	0.109133	0.897044
H2_1	H	0.318131	0.090460	0.916563
H1_1	H	0.163126	0.333668	0.250749
H2_1	H	0.037258	0.291863	0.152049
H2_1	H	0.112480	0.337446	0.099456
H1_1	H	0.601323	0.313642	0.811517
H2_1	H	0.559454	0.446002	0.717443
H2_1	H	0.476014	0.417917	0.768356
H1_1	H	0.400232	0.220587	0.846547
H2_1	H	0.495066	0.107225	0.768682
H2_1	H	0.537077	0.213901	0.773164
H1_1	H	0.218007	0.521430	0.185915
H2_1	H	0.247006	0.391378	0.285673
H2_1	H	0.260477	0.494613	0.336668
H1_1	H	0.928782	0.688278	0.521072
H2_1	H	0.982112	0.740997	0.666342
H2_1	H	0.045536	0.655327	0.631165
H1_1	H	0.976513	0.800219	0.525907
H2_1	H	0.856893	0.916768	0.550292
H2_1	H	0.925032	0.963493	0.490281
H1_1	H	0.695717	0.792508	0.055648
H2_1	H	0.724585	0.957132	0.114990
H2_1	H	0.642070	0.960234	0.045549
H1_1	H	0.839674	0.968459	0.137778
H2_1	H	0.860393	0.825379	0.042216
H2_1	H	0.907865	0.916591	0.005595
H1_1	H	0.507564	0.653819	0.104027
H2_1	H	0.365257	0.723021	0.054708
H2_1	H	0.408928	0.667189	0.975065
H1_1	H	0.757492	0.018694	0.771338
H2_1	H	0.606178	0.049240	0.809505
H2_1	H	0.646878	0.148900	0.781074
H1_1	H	0.703674	0.056844	0.315164
H2_1	H	0.749687	0.943286	0.425701

H2_1	H	0.783284	0.050541	0.455711
H1_1	H	0.612096	0.026092	0.328911
H2_1	H	0.603520	0.885673	0.227280
H2_1	H	0.517270	0.953034	0.212063
H1_1	H	0.378834	0.064440	0.530704
H2_1	H	0.512005	0.150271	0.582624
H2_1	H	0.497504	0.061838	0.643789
H1_1	H	0.060576	0.445377	0.699379
H2_1	H	0.937576	0.345505	0.732049
H2_1	H	0.015210	0.335350	0.806102
H1_1	H	0.975544	0.548820	0.604703
H2_1	H	0.047737	0.393260	0.569947
H2_1	H	0.088758	0.476507	0.516844
H1_1	H	0.877551	0.393698	0.018050
H2_1	H	0.748074	0.316263	0.946184
H2_1	H	0.821330	0.326544	0.877953
H1_1	H	0.530561	0.391129	0.937389
H2_1	H	0.520832	0.246241	0.020484
H2_1	H	0.491146	0.219759	0.921593
H1_1	H	0.492053	0.483319	0.012715
H2_1	H	0.645790	0.460365	0.063859
H2_1	H	0.630553	0.570169	0.034691
H1_1	H	0.029619	0.559114	0.406453
H2_1	H	0.900286	0.597583	0.486805
H2_1	H	0.869084	0.561557	0.390368
H1_1	H	0.347043	0.903139	0.099011
H2_1	H	0.362078	0.069926	0.055961
H2_1	H	0.320200	0.071353	0.148048
H1_1	H	0.362863	0.991361	0.897123
H2_1	H	0.483054	0.039062	0.000689
H2_1	H	0.486117	0.102796	0.917127
H1_1	H	0.086758	0.799528	0.078668
H2_1	H	0.104326	0.964745	0.032367
H2_1	H	0.090476	0.891999	0.949298
H1_1	H	0.980858	0.947370	0.098355
H2_1	H	0.091786	0.066195	0.148860
H2_1	H	0.004954	0.122401	0.111846
H1_1	H	0.999261	0.494981	0.945780
H2_1	H	0.062034	0.418676	0.074490
H2_1	H	0.980744	0.355948	0.033997
H1_1	H	0.132597	0.472521	0.115826
H2_1	H	0.219128	0.474728	0.989756
H2_1	H	0.270572	0.410831	0.061401
H1_1	H	0.000561	0.774253	0.848164
H2_1	H	0.877067	0.826424	0.932364
H2_1	H	0.961003	0.803564	0.996317
H1_1	H	0.971104	0.113453	0.995039
H2_1	H	0.879162	0.046111	0.873310

H2_1	H	0.847504	0.004931	0.960706
H1_1	H	0.064536	0.186279	0.831828
H2_1	H	0.035185	0.017034	0.859023
H2_1	H	0.129420	0.023084	0.818930
H1_1	H	0.005608	0.653218	0.346849
H2_1	H	0.040351	0.675020	0.198504
H2_1	H	0.994280	0.571617	0.204438
H1_1	H	0.080075	0.985309	0.563284
H2_1	H	0.075482	0.107870	0.454769
H2_1	H	0.041586	0.006366	0.410870
H1_1	H	0.995856	0.193270	0.545163
H2_1	H	0.030716	0.089459	0.665752
H2_1	H	0.929134	0.123425	0.665843
H1_1	H	0.957412	0.270861	0.206635
H2_1	H	0.905659	0.182122	0.324867
H2_1	H	0.002067	0.222796	0.351916
H1_1	H	0.964085	0.389499	0.296220
H2_1	H	0.074156	0.516947	0.312219
H2_1	H	0.123092	0.413215	0.306752
H1_1	H	0.403366	0.027331	0.209717
H2_1	H	0.431831	0.988372	0.360088
H2_1	H	0.343399	0.935598	0.322022
H1_1	H	0.396995	0.076676	0.707636
H2_1	H	0.414446	0.900749	0.717192
H2_1	H	0.407425	0.949700	0.812125