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Deductive molecular mechanics of four-coordinated carbon allotropes. Supplementary materials.

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Full tables of results obtained with ADAMAS package.

Optimized unit cell parameters are presented in Table S1. Mean relative deviation in fractional coordinates does not exceed 0.1%. Calculated densities, relative energies and bulk moduli, compared to the values from SACADA, are collected in Table S2.
Densities and relative energies were calculated within the *correlated* (*corr*) setting for P_m and B_m, according to the expression eq. (3) of the main text. Bulk moduli were calculated within the mean setting for the bond characteristics: P_m=1 and B_m=1. Inserting these values to the general formula eq. (2) of the main text, one arrives to the following expression for the EBB:

Table S1. *Optimized unit cell parameters, obtained within the MNDO/corr setting.*

Name	*a*, Å		*b*, Å		*c*, Å		α		β		γ	
	Calc	SACADA	Calc	SACADA	Calc	SACADA	Calc	SACADA	Calc	SACADA	Calc	SACADA
dia	2.547	2.520	2.547	2.520	2.547	2.520	60.000	60.000	60.000	60.000	60.000	60.000
cfe	2.539	2.510	2.544	2.510	6.436	6.391	78.692	78.673	78.634	78.673	60.000	60.000
cfc	2.553	2.513	2.541	2.513	8.282	8.266	90.000	90.000	90.000	90.000	120.000	120.000
SiC12	2.547	2.511	2.542	2.511	8.428	8.400	81.401	81.404	81.404	81.404	60.000	60.000
lon	2.543	2.507	2.541	2.507	4.181	4.169	90.000	90.000	90.000	90.000	120.000	120.000
cbn	2.556	2.520	4.171	4.136	4.786	4.743	96.971	96.762	105.516	105.410	90.077	90.000
cnw	2.557	2.521	4.171	4.149	9.118	9.039	90.000	90.000	90.000	90.000	90.000	90.000
dia-a	7.702	7.516	7.703	7.516	7.702	7.516	90.000	90.000	90.000	90.000	90.000	90.000
fer	3.763	3.757	6.167	6.071	6.165	6.071	70.796	70.777	72.393	71.976	72.150	71.976
lcs	4.483	4.467	4.481	4.467	4.480	4.467	109.471	109.471	109.471	109.471	109.471	109.471
4^4T32	2.542	2.520	4.927	4.856	6.434	6.357	112.477	112.452	101.430	101.430	90.000	90.000
4^4T35	2.550	2.521	4.164	4.110	4.812	4.761	106.502	106.09	90.000	90.000	90.000	90.000
4^4T86	3.427	3.417	4.716	4.661	6.065	6.017	111.516	111.394	89.912	90.000	111.490	111.504
4^4T116	2.550	2.524	3.909	3.881	5.382	5.309	98.942	99.032	90.000	90.000	109.050	108.973
4^4T124	2.567	2.517	3.824	3.822	7.986	7.936	103.888	103.932	90.000	90.000	90.002	90.000
4^7T11	5.225	5.231	5.766	5.674	6.463	6.463	90.025	90.000	90.000	90.000	113.176	113.566

$$E_m^{mean} = \frac{1}{2}(\Delta_m - 4t_m) \quad \text{(S1)}$$

Such a mean setting allows one not to consider the distance dependence of P_m and B_m. Regrouping terms in eq. (S1) so that g_m (see the definition after eq. (2)) is absorbed in the one-center energy makes eq. (S1) equivalent to eq. (3) of Ref. 18 and satisfies the conditions under which the one-center quantities are exactly hybridization independent. Otherwise, their hybridization dependence is only weak, any way.

Table S2. *Densities and relative energies, obtained within the MNDO/corr setting, and bulk moduli obtained within the MNDO/mean setting.*

Name	Density, g/cm^3		Relative energy, eV/atom		Bulk modulus, GPa	
	Calc	SACADA	Calc	SACADA	Calc	SACADA
dia	3.415	3.535	0.000	0.000	452.8	403-484
cfe	3.412	3.522	0.015	0.010	435.95	-
cfc	3.430	3.529	0.013	0.011	439.38	453.4
SiC12	3.428	3.531	0.013	0.011	439.72	474.6
lon	3.410	3.514	0.022	0.021	447.3	405-455
cbn	3.272	3.373	0.174	0.171	418.5	414-431
cnw	3.282	3.375	0.177	0.151	422.8	403-468
dia-a	1.397	1.506	1.001	1.212	195.6	160-169
fer	2.865	2.967	0.533	0.528	339.8	-
lcs	3.455	3.489	0.975	0.889	444.1	393-441
4^{4}T32	3.291	3.408	0.154	0.150	415.8	405
4^{4}T35	3.256	3.367	0.180	0.176	397.2	395-429
4^{4}T86	3.330	3.404	0.197	0.195	423.3	-
4^{4}T116	3.190	3.290	0.393	0.296	431.4	-
4^{4}T124	3.145	3.229	0.297	0.292	400.1	-
4^{7}T11	3.120	3.176	0.614	0.666	310.1	334

As an illustration of the possibilities of the ADAMAS package, we present in Figure S1 the angular dependencies of the Young moduli $E(\vec{n})$ for T- and M-carbon.

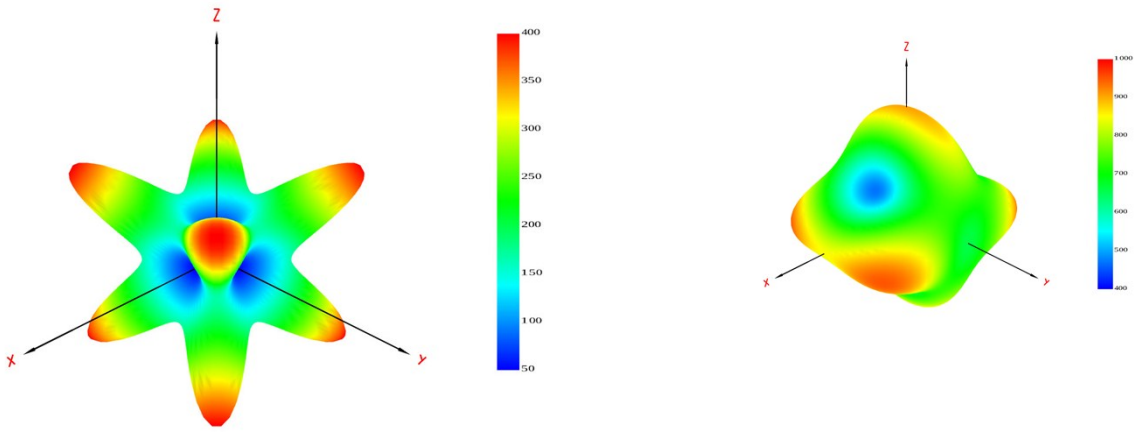

Figure S1. Angular dependence of the Young moduli of T-carbon (**dia-a** - left) and M-carbon allotrope (**cbn** - right) as calculated by the ADAMAS package.

Exemplary input for ADAMAS package.

*POSCAR file for diamond (***dia***)*

```
Diamond
1.00000
1.7827 1.7827 0.0000
0.0000 1.7827 1.7827
1.7827 0.0000 1.7827
C
2
Direct
0.0 0.0 0.0
0.25 0.25 0.25
```

dmmin file for MNDO-type parameterization with correlated (eq. (1)) treatment of densities and 4 layers of unit cells used for the core repulsion summation.

```
PARAMETERIZATION: MNDO
SLG_DENSITY: corr
BASIS_SET: STO
ORBITAL_EXPONENTS: 1.787537
RESONANCE_PARAMETERS: 0.62964 0.48650 0.34336 0.37875
NUMBER_OF_LAYERS: 4
```