Computational Details

 Input **Structures:**

- Δ: most stable elemental system (Cottenier's work: http://molmod.ugent.be/deltacodesdft and rare-earth nitrides from Topsakal-Wentzkovitch work;
- Phonon, pressure, cohesive energy: Cottenier's structures (except SiF_4 has been used for F because of convergence issues) and rare-earth nitrides;
- Bands: Cottenier's structures reduced to primitive cells (except SiF_4 has been used for F because of convergence issues) and rare-earth nitrides.

 Δ calculations:

- wave function cutoffs: 200 Ry;
- dual = 8 (PAW/US), 4 (NC);
- k-points: 20x20x20;
- smearing (degauss): Marzari-Vanderbilt, 0.002 Ry;
- non-spin-polarized calculations except Mn (antiferrimagnetic), O and Cr (antiferromagnetic), Fe, Co, and Ni (ferromagnetic).

 Phonon**, pressure, cohesive energy calculations:**

- k-points: 6x6x6, but 10x10x10 for oxygen and rare-earth nitrides;
- smearing: Marzari-Vanderbilt, 0.02 Ry;
- k-points for the isolated atoms: 1x1x1;
- smearing for the isolated atoms: Marzari-Vanderbilt, 0.1 Ry;
- unit cell for the isolated atoms: 12x12x12 Å;
- q-point: (0.5, 0.5, 0.5).
- all calculations non spin-polarized.
- note: the convergence pattern for the phonons is calculated as:

- circle = $(1/N * \sum_{i=1,N} [\omega_i(\text{cutoff}) - \omega_i(200\text{Ry})]^2 / \omega_i(200\text{Ry})^2)^{1/2} * 100$ (in percentage) and half error bar = Max $|[\omega(\text{cutoff}) - \omega(200\text{Ry})] / \omega(200\text{Ry})| * 100$, if the highest frequency is more than 100 cm^{-1};
- circle = $(1/N * \sum_{i=1,N} [\omega_i(\text{cutoff}) - \omega_i(200\text{Ry})]^2)^{1/2}$ (absolute value) and half error bar = Max $|\omega_i(\text{cutoff}) - \omega(200\text{Ry})|$, if the highest frequency is less than 100 cm^{-1};
- N is the total number of frequencies;
- For some elements, we have neglected the first n frequencies in the summation above, because the frequencies are negative and/or with strong oscillations as function of the cutoff for all the considered pseudos). We have neglected the first 4 frequencies for H and I, 12 for N and Cl, 6 for O and SiF_4 (which replaces F).

 Bands **calculations:**

- k-points for the self-consistent calculation: 20x20x20;
- k-points for the band's calculation: 6x6x6;
- smearing: Marzari-Vanderbilt, 0.02 Ry;
- all calculations non spin-polarized.