Energetics and Stability of Silicon using DFT calculations

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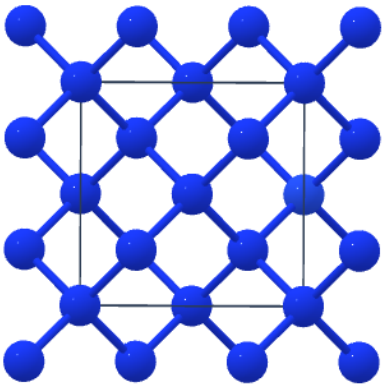

1) Let's consider the case of Si (https://materialsproject.org/materials/mp-149)

2) To extract the energy from the OUTCAR file of VASP, use the command grep "free energy" OUTCAR

3) The final (converged) value for the total energy from the Quantum Espresso simulations can be found by looking for an exclamation mark in the output file. For example, you can type the following command in the terminal: grep ! Si.sample.out (assuming that your input file is named 'Si.sample.in', then the output file should be named 'Si.sample.out').

4) **Cohesive energy (E_{coh}):** It is a measure of the stability of the material. A higher cohesive energy indicates greater stability and less likelihood of atom decomposition. The E_{coh} can be computed using the following relation:

$$E_{coh} = (E_{FCC-Si} - n \times E_{Si-atom})/n \qquad (1)$$

where, E_{FCC-Si}, $E_{Si-atom}$, and n are the total energy of the Si crystal, total energy of the isolated Si atom and the number of Si atoms in the FCC Si system, respectively.

5) **Formation energy (E_{form}):** Relying solely on cohesive energy is insufficient to determine the existence of the material. Therefore, it is recommended to compute the formation energies, along with other stability features, such as the dynamical and mechanical properties. The formation energy of Silicon can be calculated using the following equation:

$$E_{form} = (E_{FCC-Si} - n \times E_{Si-stable})/n \qquad (2)$$

where E_{FCC-Si} is the total energy of the Si system, $E_{Si-stable}$ is the total energy of a Si atom in its most stable form, and n is the number of Si atoms in the Si system.

6) **Vacancy formation energy (E_{VFE})**: The vacancy formation energy of a crystal is the energy required to create a vacancy by removing one atom from the crystal. The E_{VFE} of Si can be computed using the relation:

$$E_{VFE} = E_{defect} - E_{perfect} + n_i \mu_i \qquad (3)$$

where E_{defect} and $E_{perfect}$ are the total energies of the Si with vacancy defects and pristine surface, respectively. The n_i is the total number of Si atom vacancies and μ_i is the chemical potential of the Si atoms which are taken as the bulk energy of FCC Si.

Read more about the energy concept here:

1. https://pubs.acs.org/doi/10.1021/acsnano.6b05240 -> Estimation of Formation Energy
2. https://doi.org/10.1002/adts.202000250
3. https://doi.org/10.1039/D1CP05590A

Task 1:

How to compute the cohesive and formation energies of SiC (https://materialsproject.org/materials/mp-8062)? How do you modify the above equations for materials composed of binary and ternary elements? Compare your results with the existing literature values.