A Framework for Automating Point-Defect Calculations

Scientific Achievement

Completed and rigorously validated open-source Python framework to automate first-principles point-defect calculations.

Significance and Impact

The automated defect calculations enable large-scale predictions of materials' defect properties. Therefore, this framework provides a key tool for including defect properties into theory-guided Materials-by-Design approaches to materials development.

Research Details

- Framework provides an effective and efficient method to identify candidate interstitial structures (in addition to other point defects).
- Applies correction schemes—(a) potential alignment, (b) image-charge correction, and (c) band-filling correction to shallow defects—to rectify finite-size artifacts within the supercell approach.
- Validated by predicting point defects' formation energies and charge transition levels for representative materials (Si, ZnO, In_2O_3).

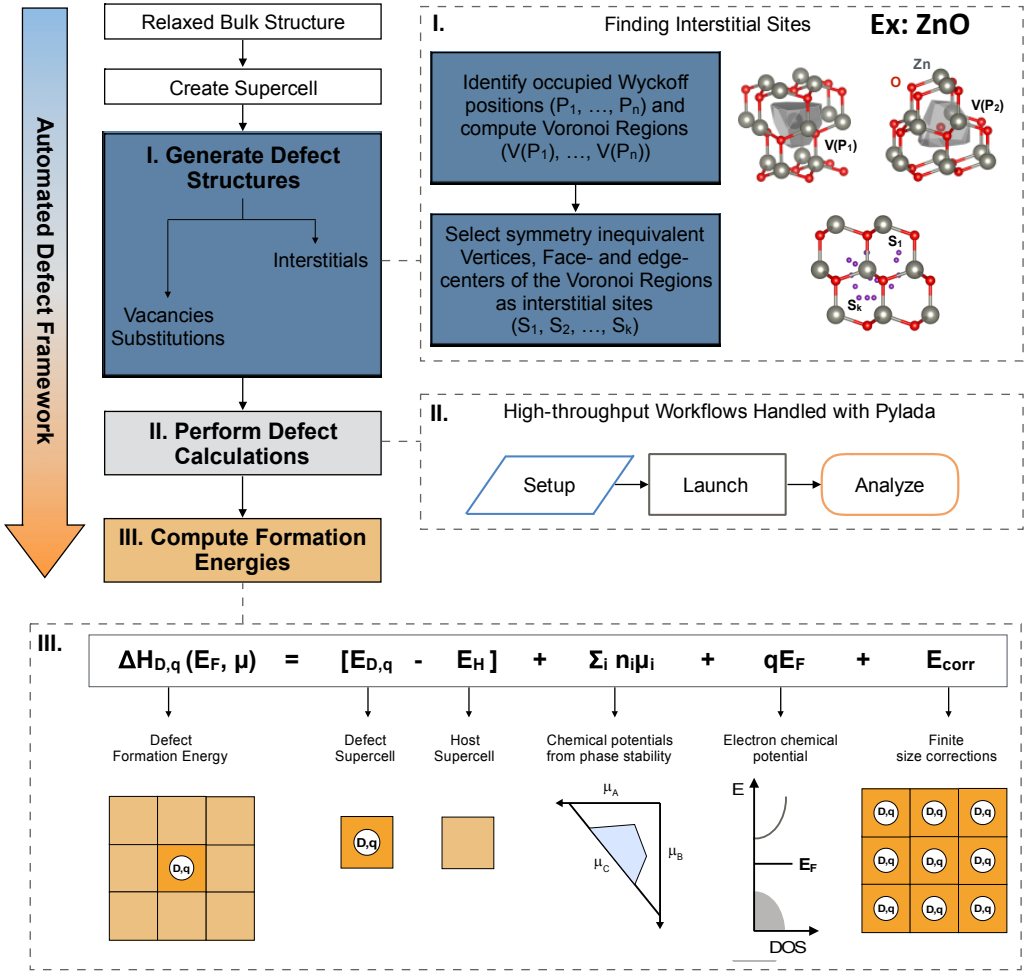

Figure 1: Overview of the automated workflow to perform point-defect calculations.

A. Goyal, P. Gorai, H. Peng, S. Lany, & V. Stevanović, *Comp. Mater. Sci.*, **130**, 1–9 (2017).

https://github.com/pylada/pylada-defects

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