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A Computational Framework for Automation of Point Defect Calculations ANUJ GOYAL[1], PRASHUN GORAI[2], Colorado School of Mines, Golden, Colorado 80401, HAOWEI PENG, STEPHAN LANY, National Renewable Energy Laboratory, Golden, Colorado 80401, VLADAN STEVANOVIC[3], Colorado School of Mines, Golden, Colorado 80401, NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, COLORADO 80401 COLLABORATION — A complete and rigorously validated open-source Python framework to automate point defect calculations using density functional theory has been developed. The framework provides an effective and efficient method for defect structure generation, and creation of simple yet customizable workflows to analyze defect calculations. The package provides the capability to compute widely accepted correction schemes to overcome finite-size effects, including (1) potential alignment, (2) image-charge correction, and (3) band filling correction to shallow defects. Using Si, ZnO and In2O3 as test examples, we demonstrate the package capabilities and validate the methodology. We believe that a robust automated tool like this will enable the materials by design community to assess the impact of point defects on materials performance.

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