Scientific Achievement

The performance of the recently developed HLE17 high-local-exchange functional was tested with a variety of solid-state materials: it was found to predict more accurate band gaps than six other local functionals and was able to localize holes as polarons, which other local functionals usually fail to do.

Significance and Impact

The HLE17 functional calculated realistic band gaps without correction terms, making computation more efficient. HLE17 can also predict realistic electronic and polaronic structures for defect systems, including some systems containing transition metals.

Research Details

The performance of HLE17 was compared to PBE, PBE+U, PBEsol, M06-L, TPSS, and HSE06.

- Lattice constants, band gaps, delithiation energies, charge carrier transition levels, and magnetic moments were calculated.
- Calculations were done using VASP and MN-VFM, a locally modified VASP module.

Seven exchange–correlation functionals were assessed for their ability (i) to predict band gaps of silicon, diamond, and Li-ion battery cathode materials, (ii) to localize hole polarons and predict delithiation energies in Li-ion battery cathode materials, and (iii) to predict transition levels of charge carriers of doped silicon and diamond.