New density functional and backflow transformation applied to Si interstitial defects

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Continued disagreement over the value of the silicon single interstitial formation energy[1] motivates continued study employing recently-developed electronic structure techniques.

The recent generalized-gradient approximation (GGA) density functional of Perdew, PBEsol,[2] restores the gradient expansion of exchange for slowly-varying densities to match the uniform electron gas limit and alters the correlation to fit the jellium surface exchange-correlation energy. With plane-wave bases and norm-conserving pseudopotentials, PBEsol lowers both the total energies of bulk and defect from its parent functional PBE by $\sim$1.5 eV per atom but increases the formation energy by an average of 0.7 eV, resulting in good agreement with calculations using the HSE functional and previous quantum Monte Carlo calculations.[3]

The inhomogeneous backflow transformation in quantum Monte Carlo improves the nodal surface of the trial wave function by modifying the electron coordinates based on interparticle distances.[4] Application of backflow in variational Monte Carlo to one defect lowers the total energies of both silicon bulk and defect by $\sim$0.1 eV per atom while keeping unchanged the formation energy within statistical uncertainty.

[1] R. Vaidyanathan *et al.*, Phys. Rev. B **75**, 195209-1 (2007).

[2] J. P. Perdew *et al.*, Phys. Rev. Lett. **100**, 136406 (2008).

[3] E. R. Batista *et al.*, Phys. Rev. B **74**, 121102 (2006).

[4] P. López-Ríos *et al.*, Phys. Rev. E **74**, 066701 (2005).