Backflow Transformation Lowers QMC Energies of a Silicon Interstitial Defect

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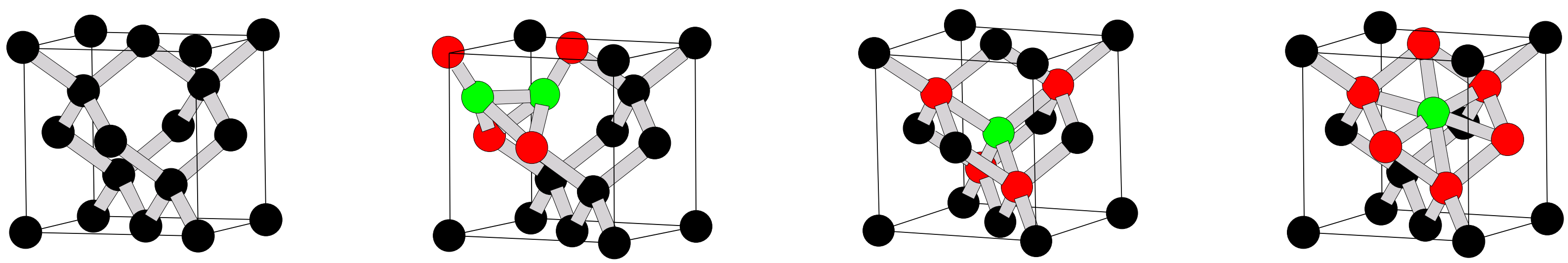
Silicon Single-Interstitial Defects



bulk **X** **T** **H**

- Extended defects enhance dopant diffusion and limit device size.
- Single-interstitial defects nucleate extended defect precipitates.

Formation Energy

$$\mathrm{E_{form}(defect) = E_{total}(defect) - \frac{N_{atoms}(bulk) + 1}{N_{atoms}(bulk)} E_{total}(bulk)}$$

QMC produces accurate Si defect formation energies.

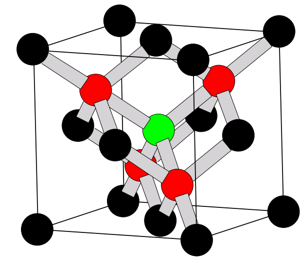
W.-K. Leung *et al.*, Phys. Rev. Lett. **83**, 2351(1999)

E. Batista *et al.*, Phys. Rev. B **74**, 121102(2006)

Outline

- Backflow transforms coordinates to better account correlation
- Hybrids incorporate Hartree-Fock exchange into DFT E_{xc}

In the silicon T defect,



- Hybrid DFT gives functional-dependent results for E_{form}:

  $E_{form}(\mathrm{PBE0}) \sim E_{form}(\mathrm{DMC})$
  $E_{form}(\mathrm{B3LYP}) \sim E_{form}(\mathrm{DMC}) + 0.9\mathrm{eV}$

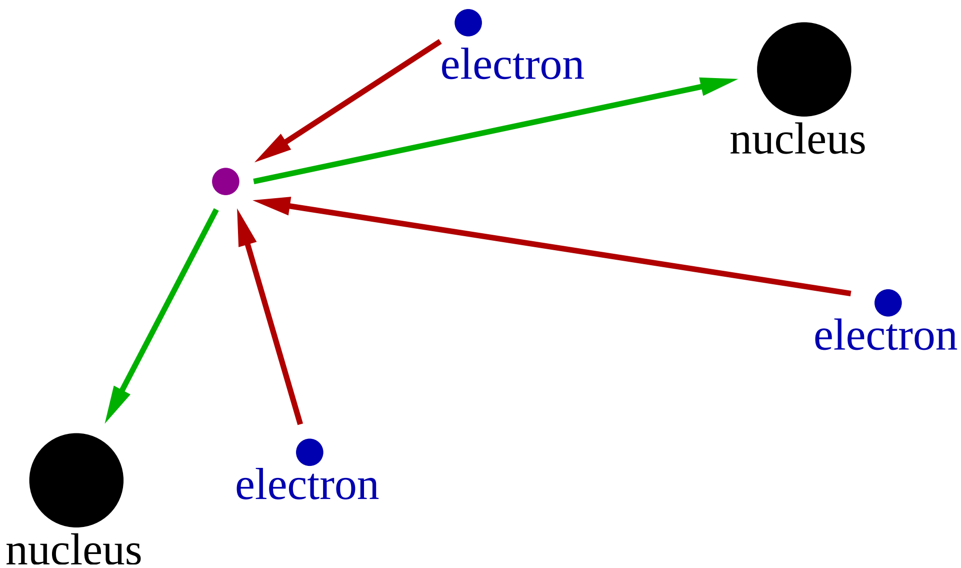
- Backflow improves VMC E_{total} but not E_{form}

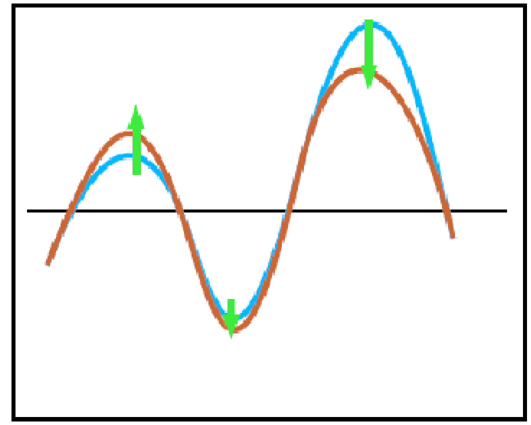
  $E_{total}(\mathrm{VMC, backflow}) \sim E_{total}(\mathrm{VMC}) - 0.6\,\mathrm{eV/atom}$
  $\sigma^2(\mathrm{VMC, backflow}) \sim \frac{1}{2}\sigma^2(\mathrm{VMC})$

Backflow transformation improves VMC E_{total} in a Si single interstitial defect.

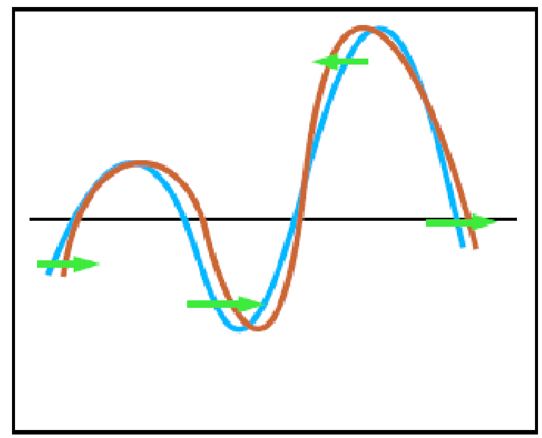
Backflow Transforms Electron Coordinates in the Slater Determinant

$$\exp(J(r_{ij}))\det\left[\phi_i\left(r_j\right)\right] \longrightarrow \exp(J(r_{ij}))\det\left[\phi_i\left(x_j\right)\right] \qquad r_i \longrightarrow x_i = r_i + \xi_i$$





Jastrow enhances Ψ_{T} magnitude



Backflow enhances Ψ_{T} nodes

Backflow : preferential displacement of electrons due to correlation; improves Ψ_{T} nodes

P. López-Ríos *et al.*, Phys. Rev. E **74**, 066701(2006)

Hybrid Density Functionals Include Hartree-Fock Exchange

HF = Hartree-Fock LDA = local-density approximation

PBE = Perdew-Burke-Ernzerhof (includes gradient of density)

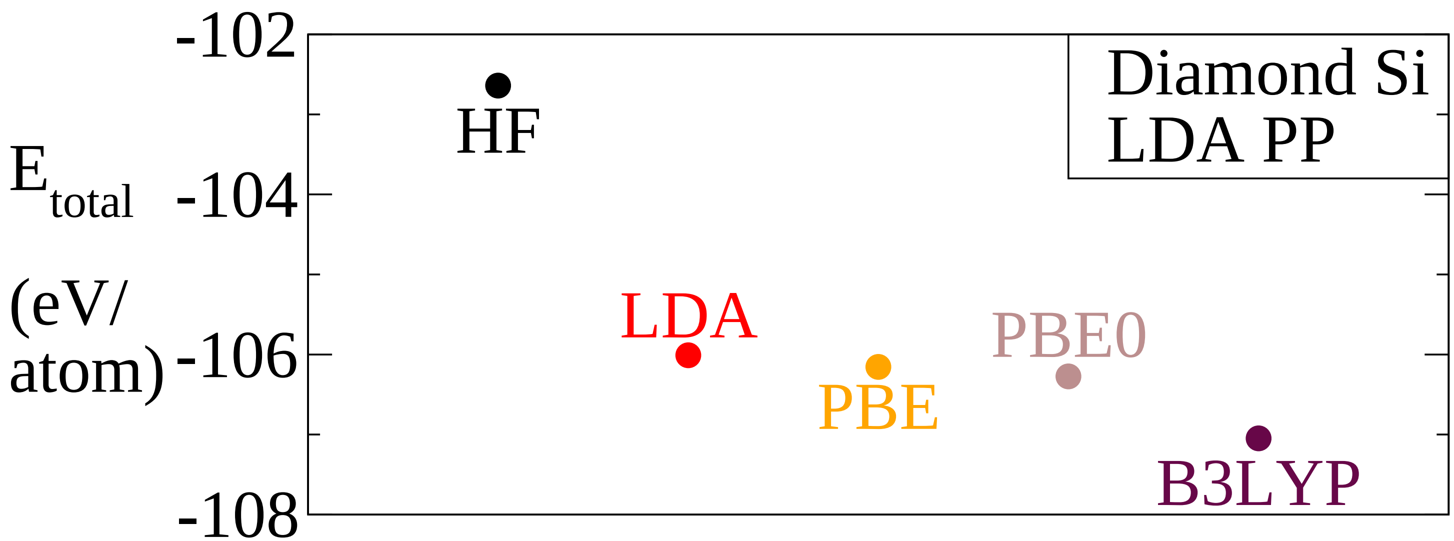
Becke's three-parameter Lee-Yang-Parr (B3LYP) functional

$$E_{xc}(\text{B3LYP}) = 0.2E_{x,\text{HF}} + 0.8E_{x,\text{LDA}} + 0.72E_{x,\text{Becke}} + 0.19E_{\text{VWN}} + 0.81E_{c,\text{LYP}}$$

Perdew-Burke-Ernzerhof hybrid (PBE0) functional

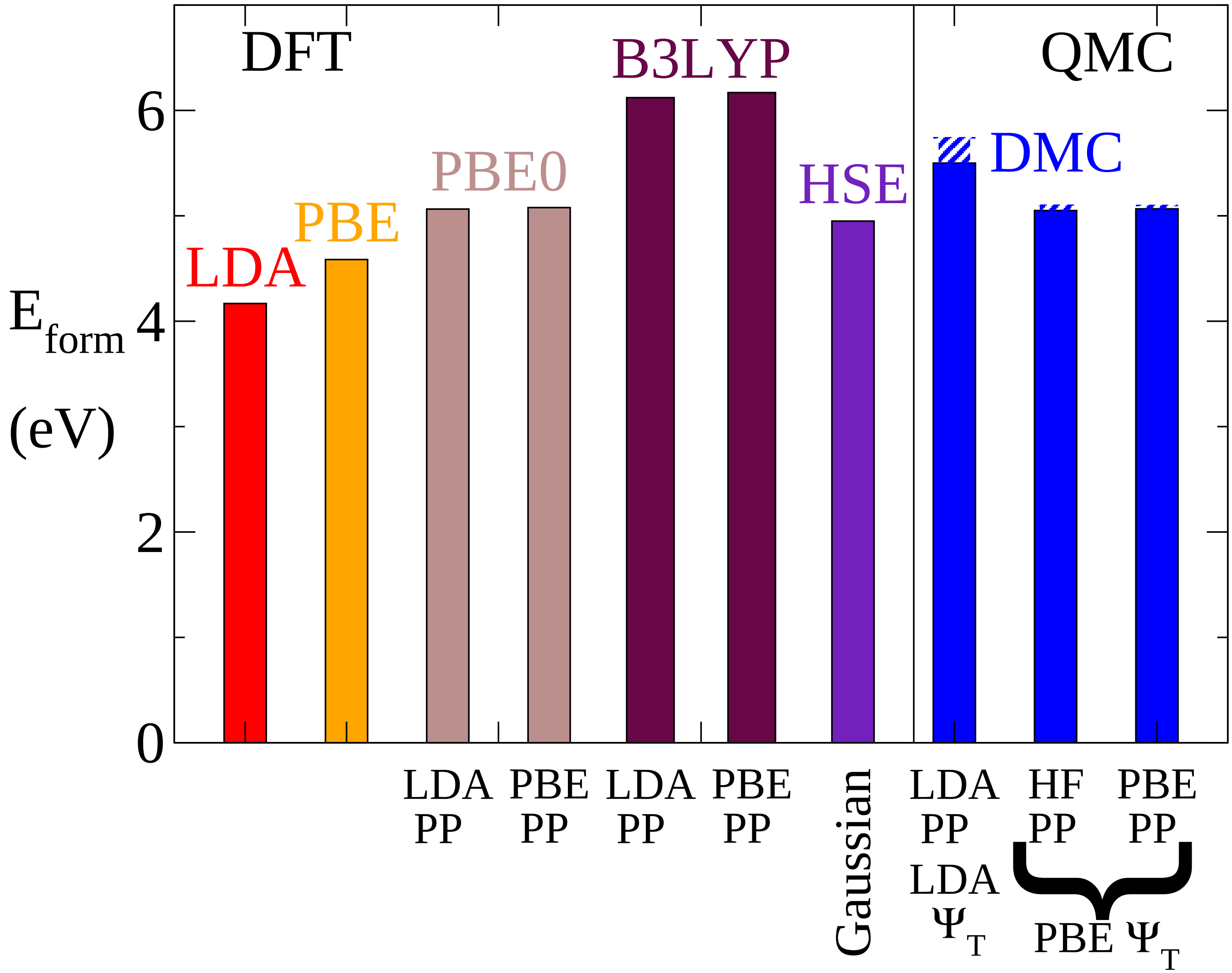
$$E_{xc}(\text{PBE0}) = 0.25E_{x,\text{HF}} + 0.75E_{x,\text{PBE}} + E_{c,\text{PBE}}$$

Hybrid screened exchange (HSE) functional = PBE0 with $E_{x,\text{HF}}$ screened at large distances



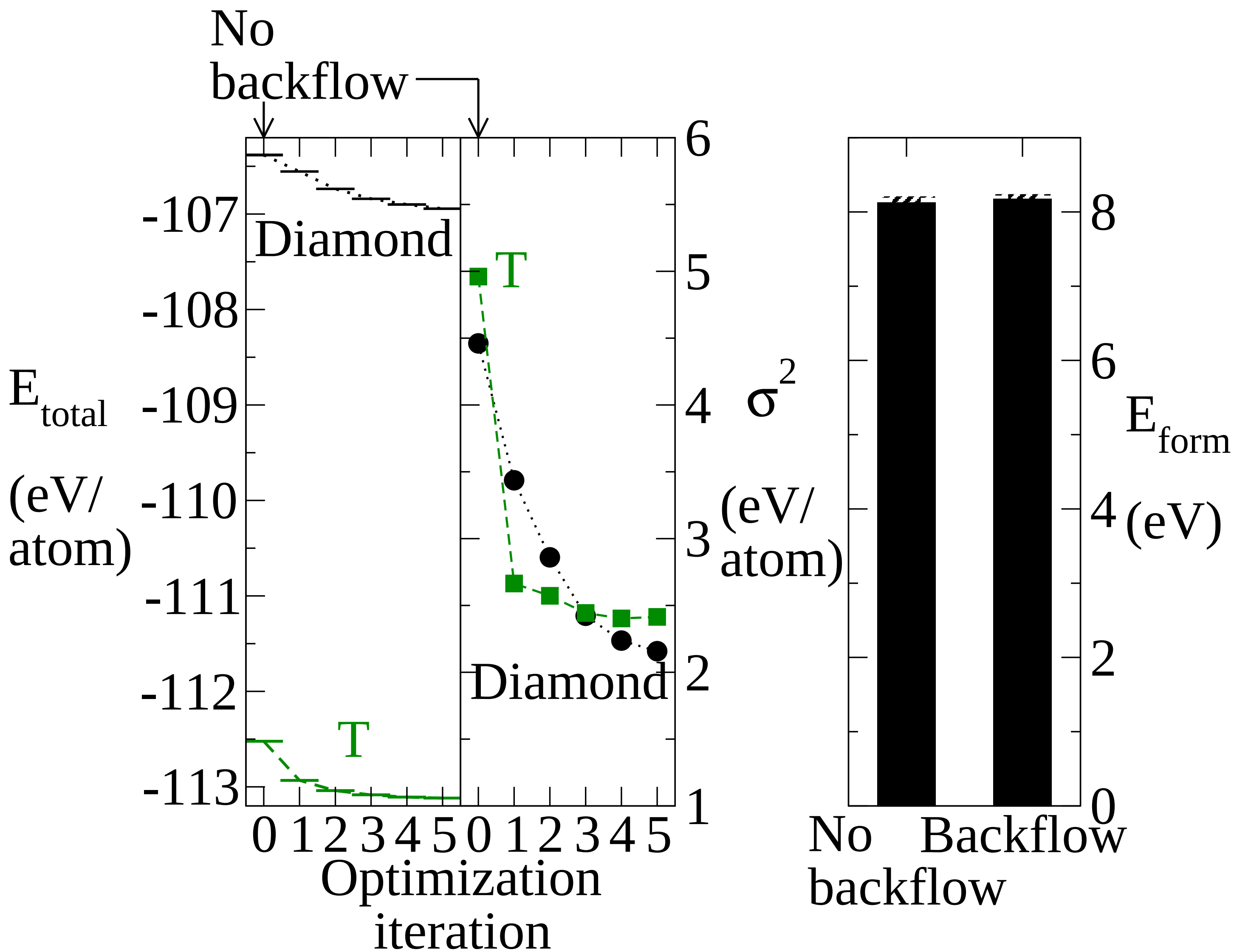
Hybrid functionals lower DFT energy.

T Defect Formation Energies in DFT



Hybrid functionals: PBE0 E_{form} close to DMC, B3LYP overshoots

T Defect Formation Energies in VMC

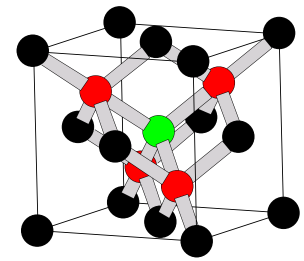


Backflow lowers $\mathrm{E}_{\mathrm{total}}$ **but does not change** $\mathrm{E}_{\mathrm{form}}(\mathrm{VMC})$

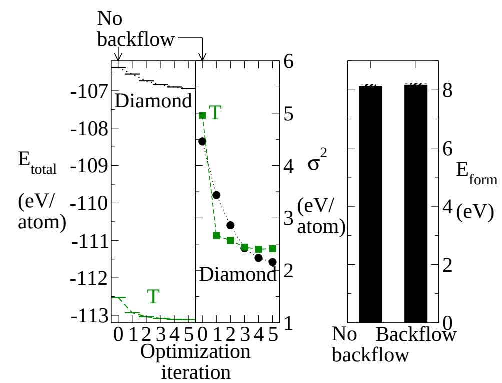
Conclusions

- Backflow transforms e^- coordinates for better correlation.
- Hybrid density functionals incorporate Hartree-Fock exchange, lowering the DFT energy.

In the silicon T defect,



- Hybrid functionals approach DMC energy irregularly
- Backflow lowers the VMC E_{total} by 0.6 eV/atom



Backflow improves VMC total energy of a Si single-interstital defect.