First-principles and empirical potential simulation study of intrinsic and carbon-related defects in silicon

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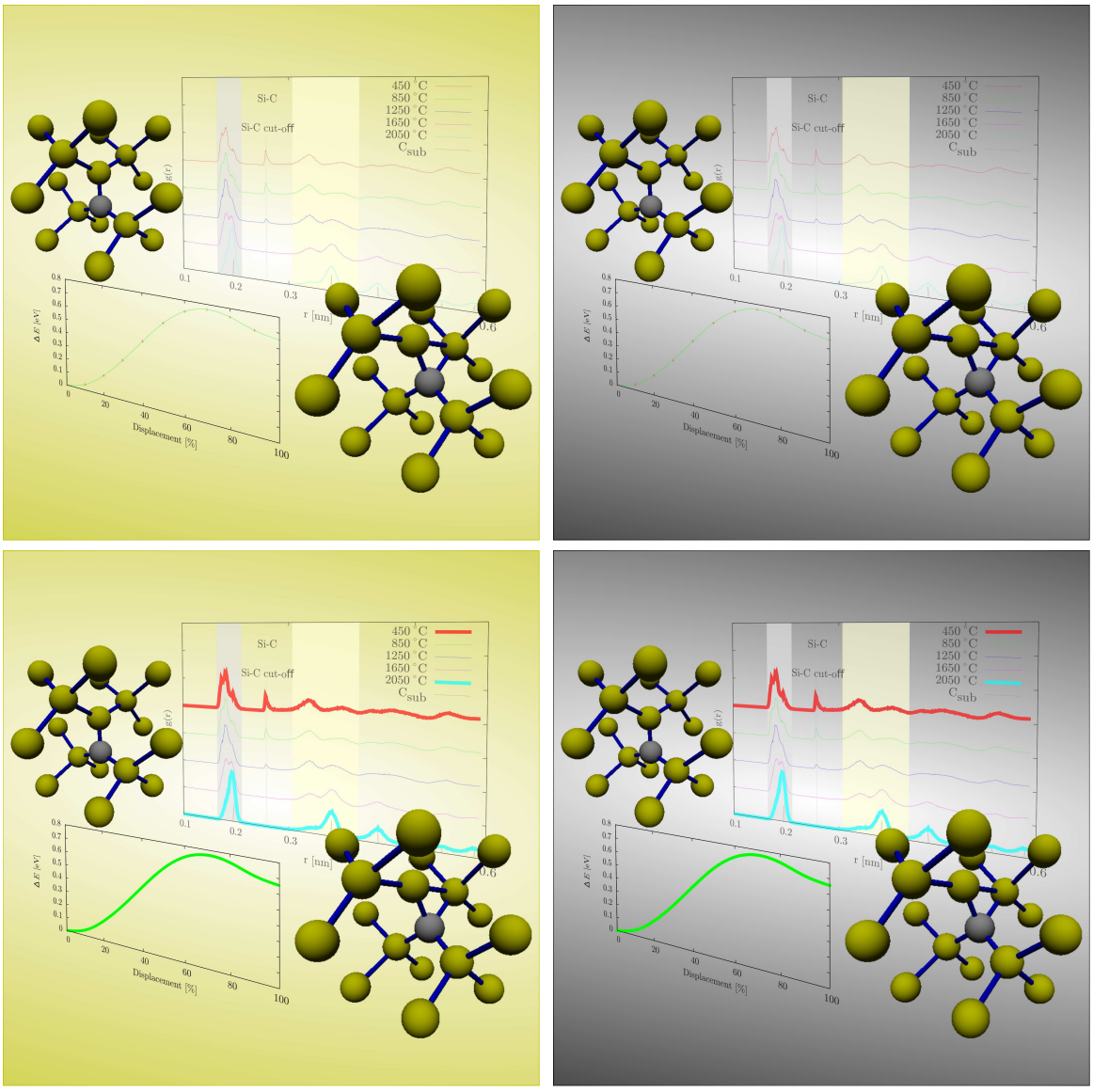

The cover page shows an initial C-Si $[0\,0\,\bar{1}]$ dumbbell configuration in bulk Si (top left) changing into a Si-Si $[1\,1\,0]$ split interstitial configuration located next to a lattice site that is substitutionally occupied by a C atom (bottom right). First-principles total energy calculations describing the energetics of this transition (front left) reveal a diffusion barrier of no more than 0.8 eV for the deviation out of the ground-state configuration. And indeed, in large systems consisting of six thousand C atoms incorporated into a Si host of a quater of a million of atoms, these transitions can be observed with increasing temperature as can be seen within the shaded regions of the radial distribution function of Si-C bonds (rear right) obtained by large-scale empirical potential molecular dynamics simulations. These results suggest an important role of substitutionally incorporated C in the silicon carbide precipitation process at elevated temperatures or far from equilibrium.