Hole trapping at Al impurities in silica: A challenge for density functional theories

The atomic geometry and electronic structure around a neutral substitutional Al impurity in silica is investigated using either the unrestricted Hartree-Fock (UHF) approximation, or Becke's three-parameter hybrid functional (B3LYP). It is found that the B3LYP functional fails to describe the structural distortions around the Al impurity, while the UHF results are consistent with experimental information. We argue that the failure of the B3LYP functional is caused by the incomplete self-interaction cancellation usually present in density functional theories.

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