Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Electronic Structure of donor pairs in Si[1] BELITA KOILLER, ANDRE SARAIVA[2], Universidade Federal do Rio de Janeiro, Brazil, MARIA JOSE CALDERON, Instituto de Ciencia de Materiales de Madrid-CSIC, Spain, FERNANDO GONZALEZ-ZALBA, Hitachi Cambridge Laboratory, Cavendish Laboratory, UK, DOMINIK HEISS, Technische Universiteit Eindhoven, Netherlands, ANDREW J. FERGUSON, Cavendish Laboratory, UK — We develop an effective mass theory for a pair of substitutional group-V donors in Si. An empirical central cell correction for a single donor, applied to energies and wavefunctions, leads to an accurate description of the D_2 "molecular" spectrum. No configuration averages simulating an ensemble of pairs are taken: our formalism applies to the single pair regime, including the A1, T and E single donor states in the hydrogenic S-like manifold and a Configuration Interaction approach to account for electron-electron correlations. We also obtain the inter donor distance dependence of experimentally accessible quantities: first ionization ($D_2^0 \rightarrow D_2^+$), second ionization ($D_2^+ \rightarrow D_2^{++}$) energies, charging energy and singlet-triplet splitting. All results are consistent with recently performed experiments on As doped Si, suggesting that our approach is reliable down to distances ~ 2 nm, and possibly smaller.

[1]Support: CNPq, FAPERJ, CAPES (Brazil), MINECO-Spain FIS2012-33521, CNPq (Brazil)-CSIC (Spain) collaboration grant.
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Date submitted: 13 Nov 2013 Electronic form version 1.4