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Atomistic configuration interaction simulations of two-electron states of donors in silicon ARCHANA TANKASALA, YU WANG, GERHARD KLIMECK, RAJIB RAHMAN, Purdue University — Two-electron states bound to donors in silicon are important for both two qubit gates and spin readout. We present a full configuration interaction technique in the atomistic tight-binding basis to capture multi-electron exchange and correlation effects taking into account the full bandstructure of silicon and the atomic scale inhomogeneity of a nanoscale device. The negatively charged two-electron D^- state of a single donor is solved as a function of a vertical field and depth from the silicon surface. Excited s-like states are found to strongly influence the charging energy. The same technique is used to solve the two-electron states of two donors as a function of separation, showing the transition from a Heitler-London like regime to a molecular regime. Excited valley states are found to affect the exchange energy for small donor separations.

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