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Atomistic simulations of energy levels in silicon quantum dots for spin filling experiments[1] RAJIB RAHMAN, RICHARD MULLER, MALCOLM CARROLL, Sandia National Laboratories, Albuquerque, NM 87185, USA — Unknown valley splitting magnitudes in enhancement-mode metal-insulator-oxide (MIS) quantum dots combined with the potential of valley-orbit coupling due to imperfect interfaces leads to complex single and multi-electron energy level dependence on magnetic and electric field strengths. Comparable energy spacing between orbital energies and the upper bands in unstrained silicon, split off because of differences in effective mass, introduce additional potential complexity. Addition energy and spin filling experiments provide a fingerprint of these energy levels for which accurate models are invaluable. Using atomistic simulations, we obtain theoretical valley-orbit splittings in silicon dots with different barrier materials, electric and magnetic fields. The multi-valley structure of Si gives rise to degenerate orbital states, which can be split by the valley-orbit interaction. The results illuminate the role of Hund's rules and valley degrees of freedom on the few electron states of the dots.

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