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Quantum size effects in competing charge and spin orderings of dangling-bond wires on Si(001)[1] JUN-HYUNG CHO, Hanyang University & The University of Tennessee, JI YOUNG LEE, Hanyang University, ZHENYU ZHANG, Oak Ridge National Laboratory & The Univeristy of Tennessee — Using spin-polarized density functional theory calculations, we investigate the competition between charge and spin orderings in dangling-bond (DB) wires of increasing lengths fabricated on an H-terminated Si(001) surface. For wires containing less than 10 DBs as studied in recent experiments, we find antiferromagnetic (AF) ordering to be energetically much more favorable than charge ordering. The energy preference of AF ordering shrinks in an oscillatory way as the wire length increases, and preserves its sign even for DB wires of infinite length. The oscillatory behavior can be attributed to quantum size effects as the DB electrons fill discrete quantum levels. The predicted AF ordering is in startling contrast with the prevailing picture of charge ordering due to Jahn-Teller distortion or Peierls instability for wires of finite or infinite lengths, respectively.

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