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Magnetism of silicon doped with alkaline earth elements BANG-GUI LIU, Department of Physics, University of California at Berkeley, and the Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, LI-JIE SHI, Institute of Physics & Center for Condensed Matter Physics, Chinese Academy of Sciences, Beijing 100080, China, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley, and the Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — It would be highly desirable to fashion spintronic materials based on silicon because of the vital importance of silicon in semiconductor technology. Since it is very difficult to experimentally dope transition metals into silicon, we explore the possibility of ferromagnetism in silicon doped with alkaline earth atoms using first-principle calculations. It is found that the energy needed for doping a calcium atom into silicon is approximately equivalent to the formation energy of a vacancy in silicon. Neither silicon nor any alkaline earth metal alone is magnetic, but our calculations indicate that ferromagnetism may be obtained by appropriately doping silicon with alkaline earth atoms such as calcium. This is intriguing for basic understanding of magnetism and for possible future applications.

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