PHYSICAL REVIEW B

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ERRATA

Erratum: Formation energies, binding energies, structure, and electronic transitions of Si divacancies studied by density functional calculations [Phys. Rev. B **74**, 205208 (2006)] *(1 page)* . . . . . 199901(E)
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Erratum: Scattering matrix method for multimode electron transport through quantum wires under a local magnetic field modulation and spin-orbit interaction [Phys. Rev. B **74**, 195332 (2006)] *(2 pages)* . . . . . 199902(E)
Lebo Zhang, Feng Zhai, and H. Q. Xu

Erratum: First-principles calculation of the spin-orbit splitting in graphene [Phys. Rev. B **75**, 121402(R) (2007)] *(1 page)* . . . . . 199903(E)
J. C. Boettger and S. B. Trickey