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Progressive changes in surface structure and electronic properties on Si(001) surface by CaF_2 adsorption

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Ab initio calculations, based on pseudopotentials and density functional theory, have been performed to investigate the atomic geometry and electronic structures of calcium fluoride (CaF_2) on the Si(001) surface. We have considered the experimentally observed (2×1) and (3×1) reconstructions with different bonding configurations of the CaF_2 molecule on the Si (001) surface. Our total energy calculations suggest that the (3×1) structure is slightly more preferable than the (2×1). The key structural parameters and electronic surface properties of their most stable structures have been discussed. In contrast to the experimental results, the most stable structures contain an appreciable bonding nature between the surface Si and F atoms, however, no real bonding between Si and Ca atoms is indicated.

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D. Loretto, F. M. Ross, and C. A. Lucas, Appl. Phys. Lett. **68**, 2363 (1996).

H. Ishiwara and T. Asano, Appl. Phys. Lett. **40**, 66 (1982).

R. W. Fathauer and L. J. Schowalter Appl. Phys. Lett. **45**, 519 (1984).

L. J. Schowalter, R. W. Fathauer, R. P. Goehner, L. G. Turner, R. W. DeBlois, S. Hastimoto, J. L. Peng, M. Gibson, and J. P. Krusius, J. Appl. Phys. **58**, 302 (1985).

D. Rieger, F. H. Himpsel, U. O. Karlsson, F. R. McFeely, J. F. Morar, and J. A. Yarmoff, Phys. Rev. B **34**, 7295 (1986).

R. M. Tromp and M. C. Reuter, Phys. Rev. Lett. **61**, 1756 (1988).

J. Zegenhagen and J. R. Patel, Phys. Rev. B **41**, 5315 (1990).

L. Pasquali, S. M. Suturin, V. P. Ulin, N. S. Sokolov, G. Selvaggi, A. Giglia, N. Mahne, M. Pedio, and S. Nannarone, Phys. Rev. B **72**, 045448 (2005).

J. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).

G. B. Bachelet, D.R. Hamann, and M. Schlüter, Phys. Rev. B **26**, 4199 (1982).

A. W. Munz, Ch. Zeigler, and W. Gopel, Phys. Rev. Lett. **74**, 2244 (1995).

A. Z. Alzahrani and G. P. Srivastava, Phys. Rev. B **77**, 235320 (2008).

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