Diffusion of an adsorbed Si atom on the Si(111)-(7×7) surface

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We present first-principles calculations that provide a detailed diffusion picture of an adsorbed Si atom on the Si(111)-(7×7) surface. Several diffusion paths for the adsorbed Si atom are established by mapping out the total energy as a function of its positions on the surface. For diffusion between the faulted and unfaulted halves, the energy barriers range from 0.96 to 1.21 eV, while remarkable low-energy barriers from 0.3 to 0.7 eV are discovered within the faulted and unfaulted regions.

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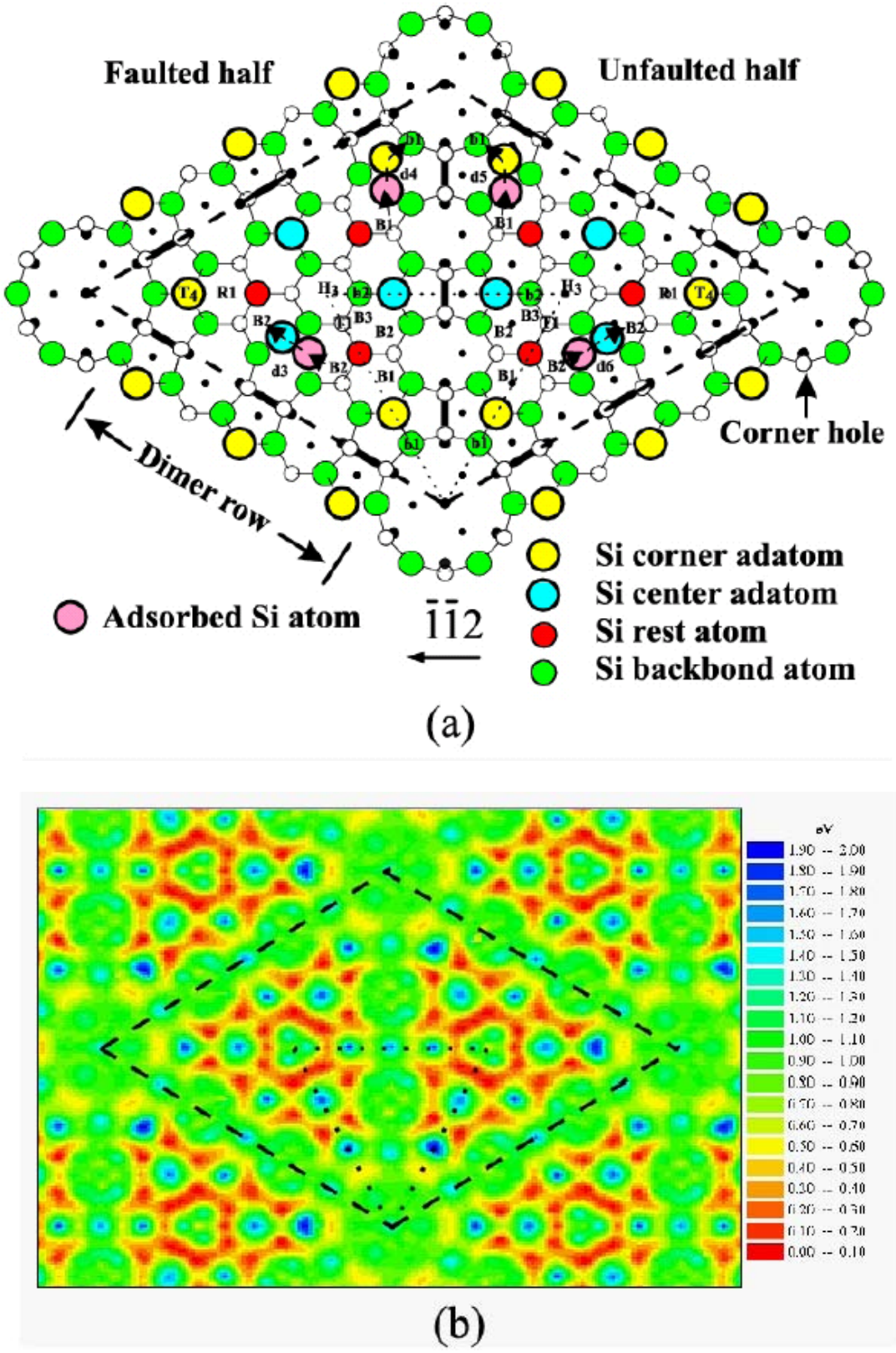

FIG. 1. (a) Top view of the DAS model of the Si(111)-(7×7) surface with four major regions. (b) The potential-energy surface for an adsorbed Si atom on the Si(111)-(7×7) surface. The (7×7) unit cell is indicated by the dashed lines.