Electronic Supplementary Information (ESI) for RSC Advances

Hydrogen solubility and diffusivity at $\Sigma 3$ grain boundary of PdCu

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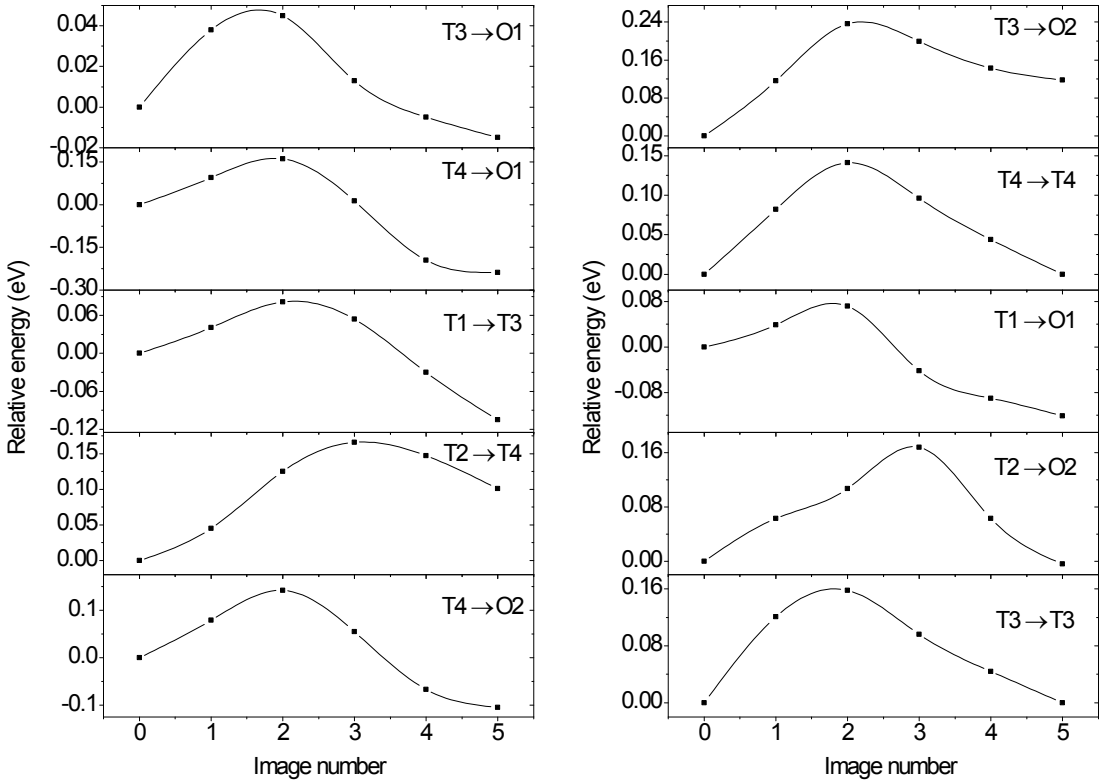

Fig. 1. The CI-NEB profile for all diffusion paths in BCC PdCu $\Sigma 3$ (112) GB without the correction of ZPE.

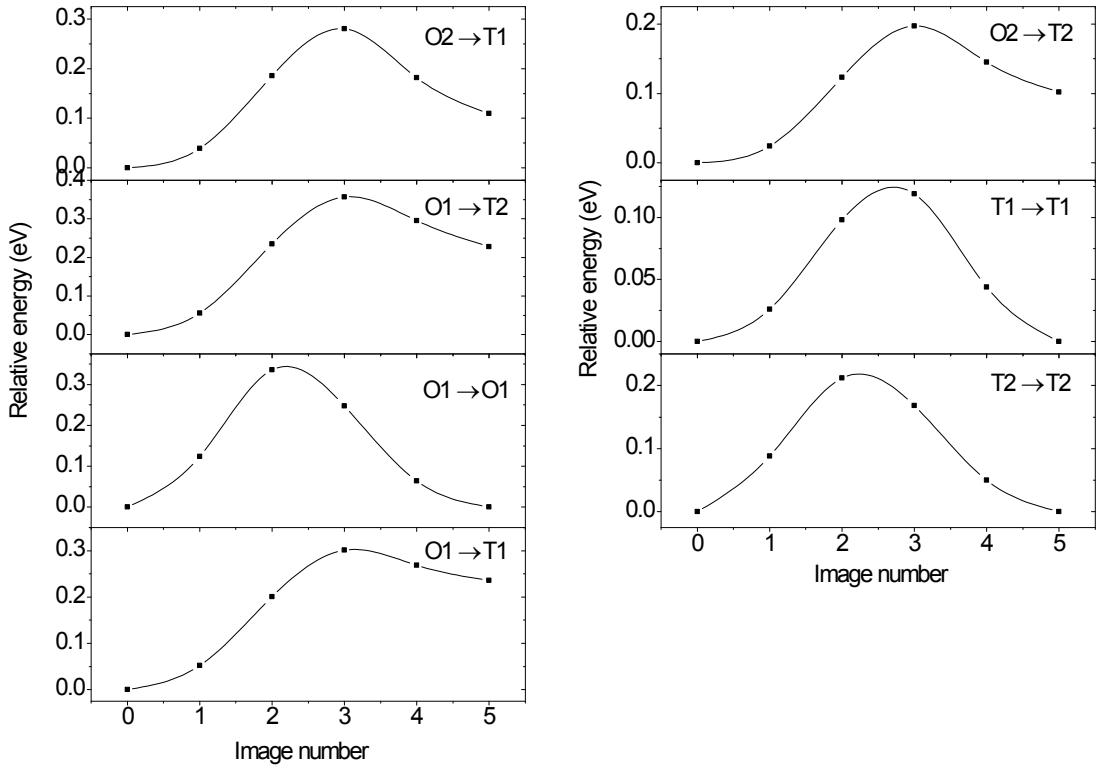

Fig. 2. The CI-NEB profile for all diffusion paths in FCC PdCu $\Sigma 3$ (111) GB without the correction of ZPE.

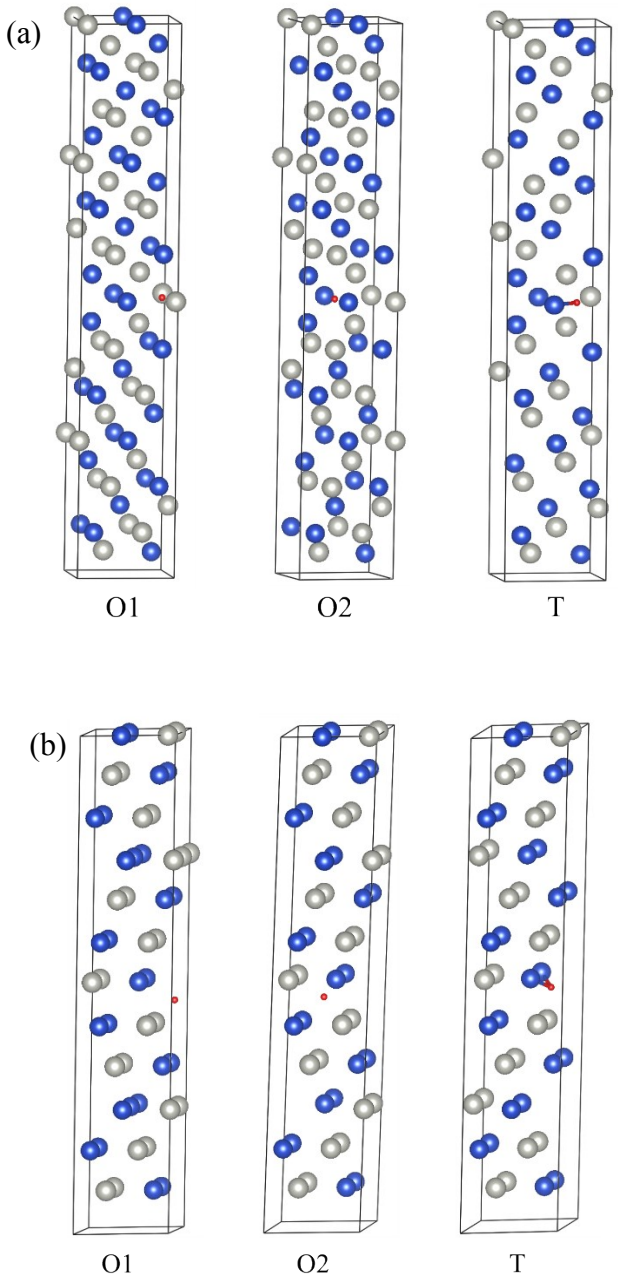

Fig. 3. The relaxed structures of H atom in (a) BCC Σ3 (112) GB and (b) FCC Σ3 (111) GB. The gray, blue and red spheres represent Pd, Cu and H atoms, respectively.

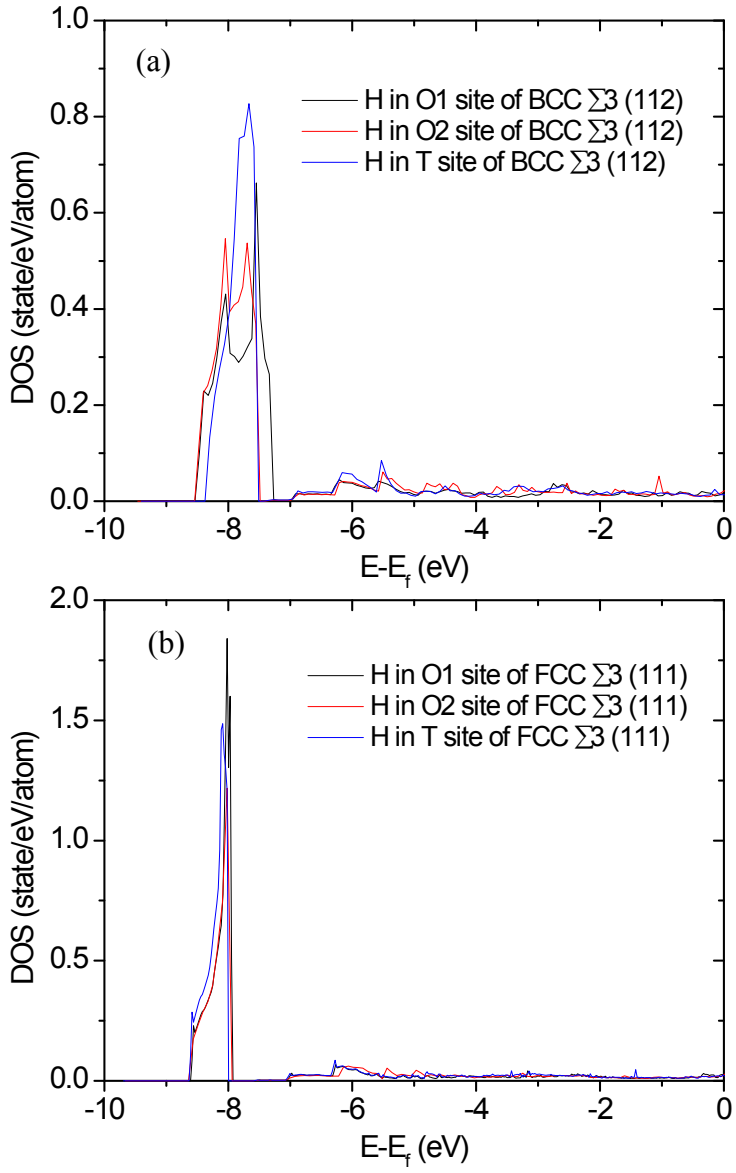

Fig. 4. The total densities of states (DOS) of H atom at the interstitial site of (a) BCC PdCu Σ3 (112) GB and (b) FCC PdCu Σ3 (111) GB.