Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Tin deposition on ruthenium and its influence on blistering in multi-layer mirrors

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1 Projected Density of States (PDOS)

Figure S2 shows the PDOS for the surface atoms on the Ru(0001) slab with and without Sn and H. The difference between the top (Ru slab) panel and the second (⅔ ML Sn on Ru) suggests metallic bonding. Sn has $5s^2p^2$ occupation. There is little change from the second (⅔ ML Sn on Ru) panel to the third (H & ⅔ ML Sn on Ru). The presence of the H layer in the fourth (⅔ ML Sn & 1ML H on Ru) panel has resulted in Ru d-H s bonding states around −7.0 eV.

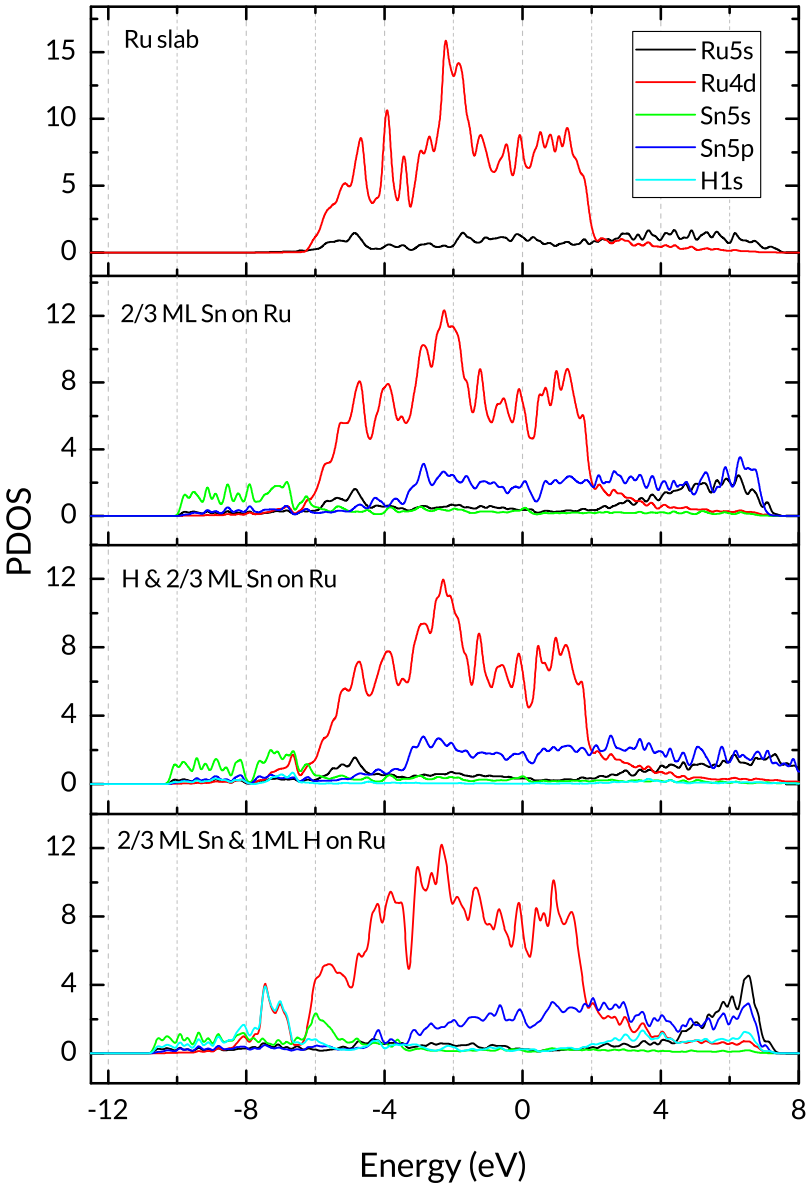
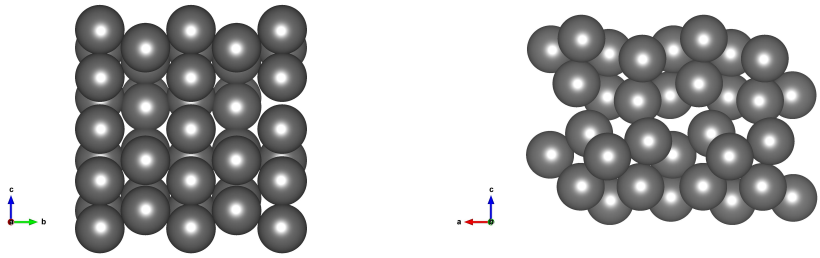


Figure S1 PDOS for (a) surface Ru atoms in Ru slab, (b) surface Ru atoms and ⅔ML Sn on Ru, (c) surface Ru atoms, ⅔ML Sn and H, and (d) surface Ru atoms, 1ML H (6 H atoms) and ⅔ML Sn. Energies are given relative to E_F at 0 eV.

2 Free Sn slabs

The 4-layer Sn overlayer slab was put through geometry optimisation without the Ru substrate. This free Sn slab has an energy of −3.67 eV/atom, against −3.68 eV/atom for a β-Sn(001) slab. The energy difference is small, which indicates minimal strain.

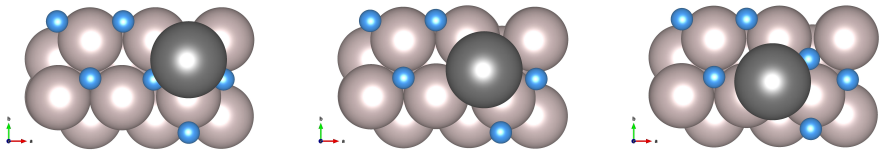


(a) β-Sn(001) slab; −3.68 eV/atom

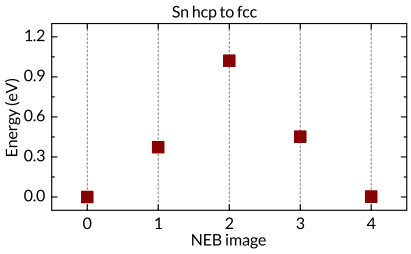
(b) Sn multilayer without Ru substrate; −3.67 eV/atom

Figure S2 Sn slabs after geometry optimisation.

3 Minimum energy paths for transition state calculations

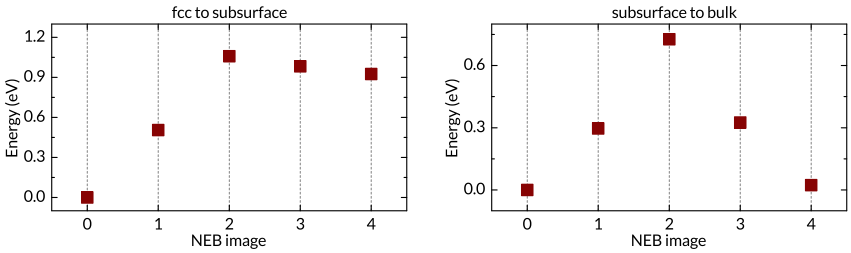


(a) Initial state **(b)** Transition state **(c)** End state



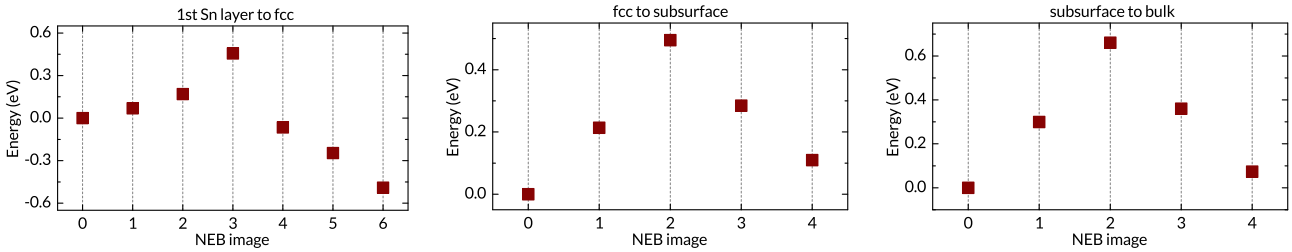
(d)

Figure S3 (a) Minimum energy path of Sn atom from *hcp* site to *fcc* site on H/Ru(0001); (b)-(d) NEB images 0, 2, and 4 respectively.



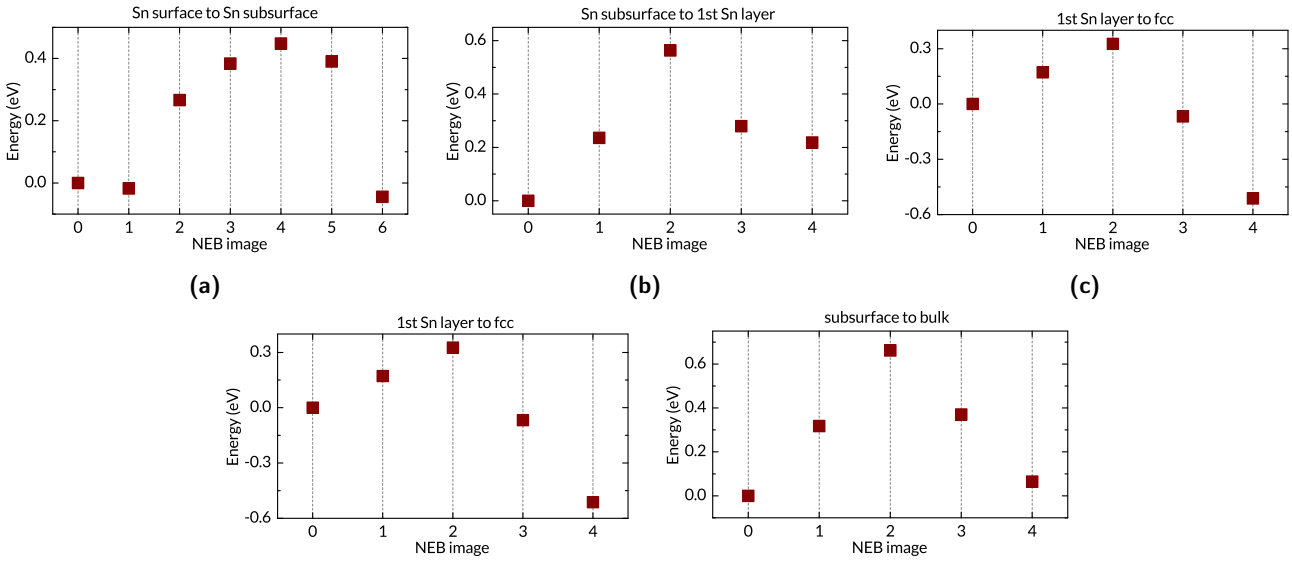
(a) (b)

Figure S4 Minimum energy paths for H diffusion on clean Ru



(a) (b) (c)

Figure S5 Minimum energy paths for H diffusion on ⅔ML Sn on Ru



(a) (b) (c)

(d) (e)

Figure S6 Minimum energy paths for H diffusion on 2ML Sn on Ru