IX Workshop on novel methods for electronic structure calculation

On the interaction of H2X molecules with the Al2C layer (X = O, S, Se, Te). A DFT study

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Introduction

- Density functional theory (PBE-GGA and HSE06), has been applied to study the adsorption of H2X molecules on the Al2C monolayer, with X = O, S, Se, Te
- The potential use of the Al2C monolayer as a sensor and a catalyst of the small molecules H2O, H2S, H2Se and H2Te was studied
- Adsorption and dissociation energies were calculated.
- The density of states (DOS) of the pristine Al2C surface and the Al2C surface with adsorbed H2O was calculated.
- The activation energies required for the dissociation processes H2X → HX + H and HX → H + X will be calculated, using the NEB (Nudged Elastic Band) and cNEB (Climbing NEB) methodology.

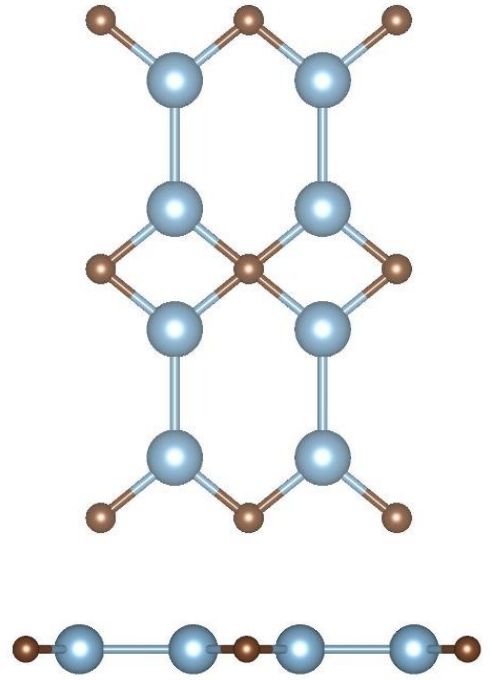

Figure 1. Al2C monolayer. Top and lateral view. A 2x2 unit cell was used with lattice constants of 6,019 and 10.14 Å

Methodology

- Vienna Ab initio Simulation Package (VASP) was used.
- The projector augmented wave (PAW) was used. Energy cut off was 450eV.
- An orthorhombic supercell with lattice constants: a =6,019 , b =10,14 and c =15 ˚A was used.
- Atomic relaxations were considered converged when all three components of the forces on the ions were less than 0.01 eV/˚A.
- The first Brillouin zone of the supercell was sampled with a (5×3×1) Γ centered mesh.

Results

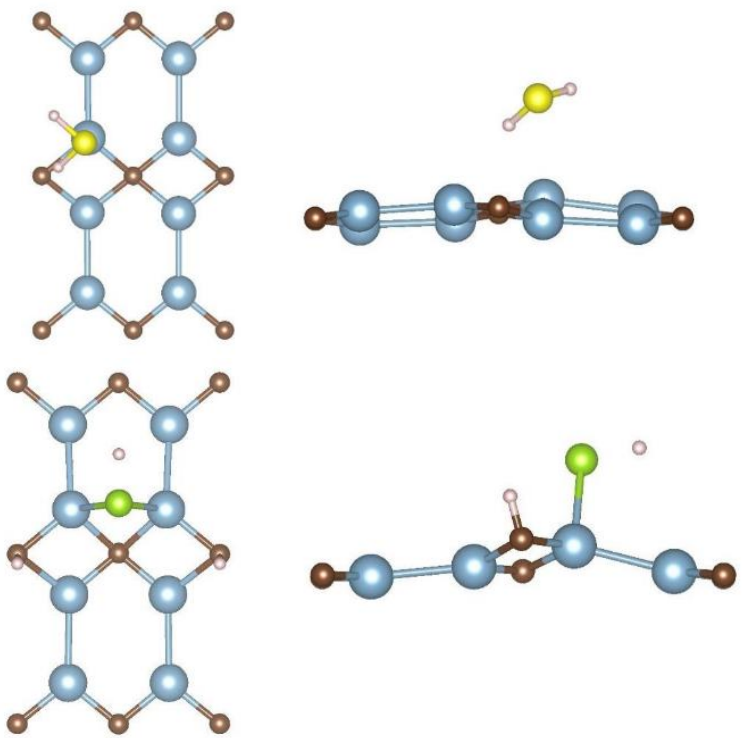

Figure 2. H_2S adsorption and H_2Se dissociation. Top and lateral views. Yellow, green and pink spheres represent S, Se and H atoms.

Table 1. Adsorption configurations of Al2C-H2X

System	Edis PBE (eV)	Angle H2X (°)	Bridge H-X (A)	Dist. Al-X (A)	Dist. C-H (A)
Al2C-H2O	-0,5096	105°	1 y 0.97	2.1	2.18
Al2C-H2S	-0.1575	91°	1.38 y 1.37	2.8	2.33
Al2C-H2Se	-0.2214	90°	1.5 y 1.48	2.81	3.49
Al2C-H2Te	-0.2963	88°	1.71 y 1.68	2.99	3.38

Table 2. Dissociation configurations of Al2c-H2X

System	Eads PBE (eV)	Bridge H-X (A)	Dist. Al-O (A)	Dist. C-H (A)
Al2C-H2O	-1,4219	0,97	1,76	1,12
Al2C-H2S	-1.699	1.35	2.46	1.14
Al2C-H2Se	-1.869	1.49	2.6	1.12
Al2C-H2Te	-1,9019	1.68	2.83	1.15

- The dissociative adsorption of the H2X molecules have the lowest energy. However, for H2S and H2O, this dissociation must be forced, because H2O and H2S interact with the Al2C surface through molecular adsorption and not direct dissociation.

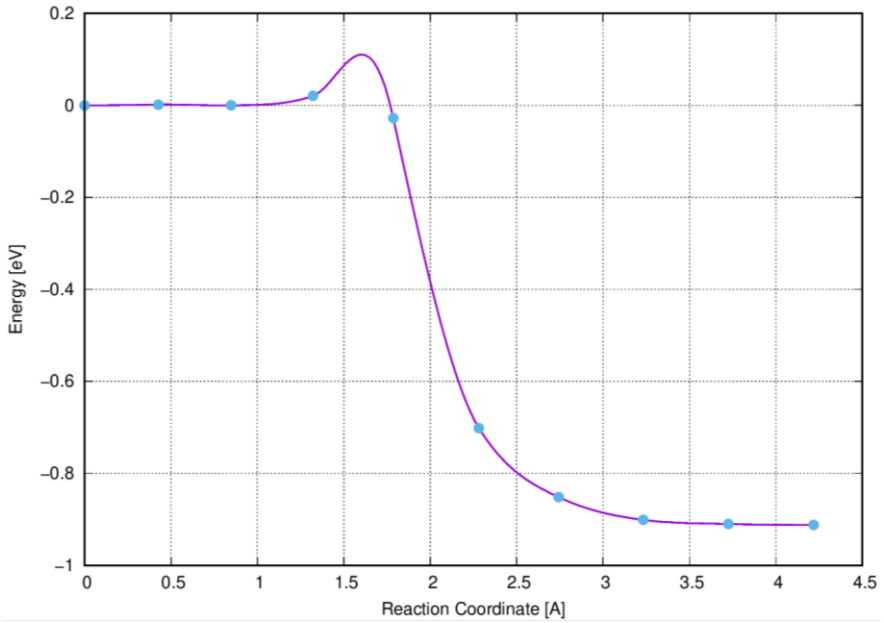

Figure 3. Al2C-H2O NEB

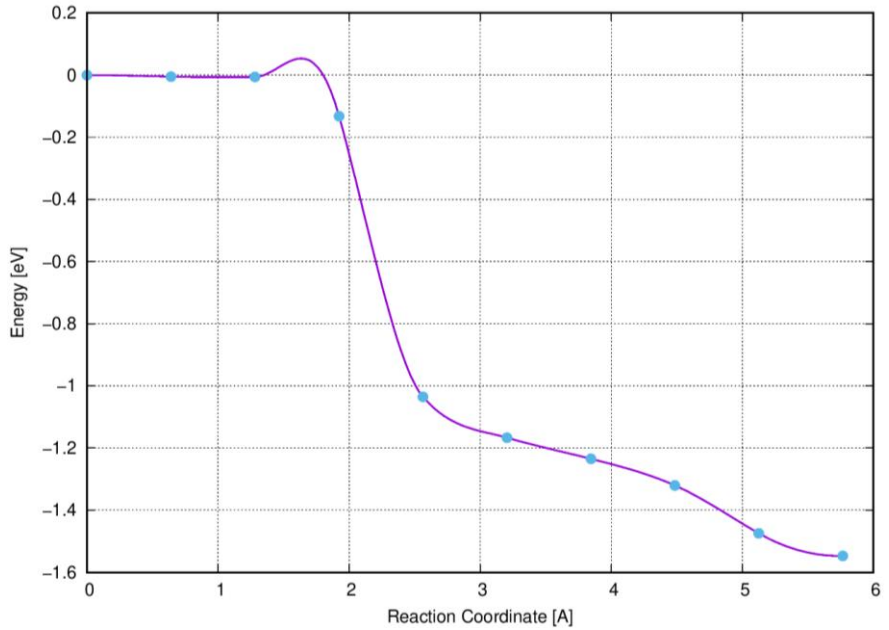

Figure 4. Al2C-H2S NEB

- The energy gaps found were 1.08 and 1.4 eV for the pristine surface and the surface with H2O adsorbed, respectively, which represents a variation of 30% if the two systems.
- The preliminary results of NEB calculations showed that the energy required to reach the transition state is approximately 0.1 eV above the adsorption energy.
- To conclude this presentation, following these preliminary theoretical results, we can say that the Al2C surface has a potential use in catalysis and as a sensor of the studied molecules: H2O, H2S, H2Se and H2Te.

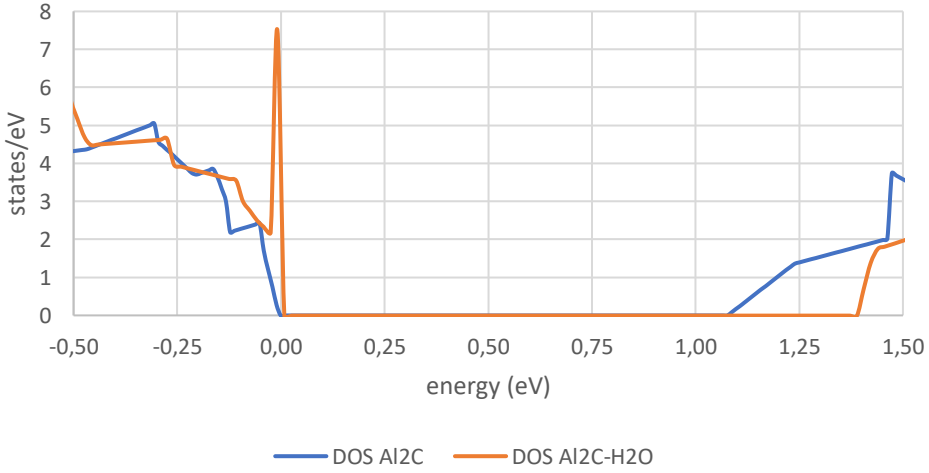

Figure 5. DOS of the pristine Al_2C and Al_2C-H_2O systems. Hybrid functional HSE06 was used