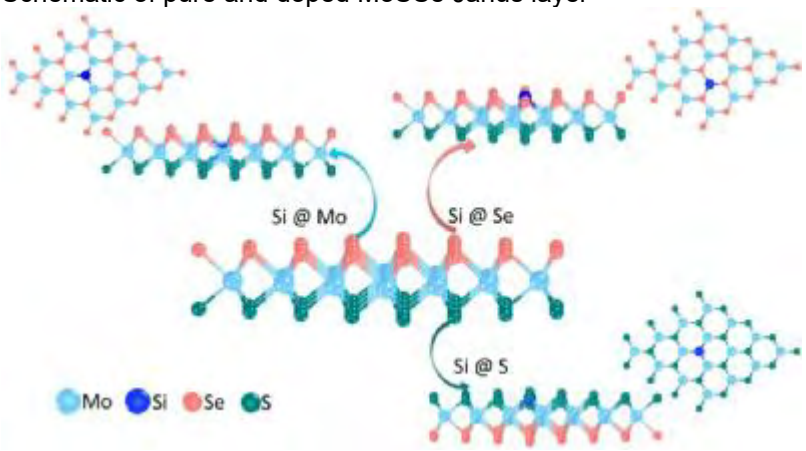
MS14-2-4 Influence of Si on hydrogen adsorption in SMoSe Janus host layer
#MS14-2-4

M. Vallinayagam [1], K. Jeyakumar [2], Z. Mattias [1], P. Matthias [3]
[1]TU Freiberg - Freiberg (Germany), [2]Rajiv Gandhi Institute of Petroleum Technology - Jais (India), [3]Helmholz Zentrum Dresden Rossendorf - Dresden (Germany)

Abstract
H adsorption on SMoSe Janus layer (JL) is enhanced by doping with Si dopant. The formation energy calculation reveals possibility of Si doing in SMoSe JL. Different sites are considered for Si doping, namely a) Si on Mo site (Si@Mo), b) Si on S site (Si@S), c) Si on Se site (Si@S), and d) Si on interstitial site (Si@int). The Si occupation on Mo sites is exothermic within Si-bulk chemical condition. Also doping on other sites, such as S or Se sites, are endothermic reaction with energy requirement about 0.4 eV. Careful analysis of the differential charge of each atom in Si-doped JLs paves the way to select possible sites for H inclusion. In the pristine JL layer the differential charge of both S and Se atoms is zero due to the uniform distortion of S-Mo and Se-Mo bond length. In Si@Mo case, the S and Se atoms in the first-nearest neighbour distance to Si acquire excess charge. On the other hand, Si@S and Si@Se cases induce no differential charge on S- or Se- atomic planes. All together lead to different choices for H adsorption sites, two sites in each S- and Se-atomic planes and top of doped element. The difference in Gibbs Free energy DG for H adsorption at different sites is calculated and compared with DG of H and H2. In conculsion, Si@Mo JLs are best candidate for H adsorption processes over pristine, Si@S and Si@Se JLs.

Schematic of pure and doped MoSSe Janus layer



Gibbs free energy of H adsorption on Janus layer