Influence of Si on Hydrogen adsorption in SMoSe Janus host layer

M. Vallinayagam[1], J. Karthikeyan[2], M. Zschronak[1] and M. Posselt[3]

[1]Institute of Experimental Physics, TUBAF, Freiberg, Germany, [2]RGIPT, JAIS, India, [3]Institute for Ion Beam physics and Materials Research, HZDR, Dresden, Germany

H adsorption on SMoSe Janus layer (JL) is enhanced by doping with Si dopant. The formation energy calculation reveals the possibility of Si doping in the 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. Doping on other sites, such as S or Se sites, are endothermic reactions with energy requirements of 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 the Si@Mo case, the S and Se atoms in the first-nearest neighbor distance to Si acquire excess charge. On the other hand, the Si@S and Si@Se cases induce no differential charge on S- or Se- atomic planes. Altogether, this leads to different choices for H adsorption sites, two sites in each S- and Se- atomic planes and on top of the doped element. The difference in Gibbs Free energy ΔG for H adsorption at different sites is calculated and compared with ΔG of H and H_2. In conclusion, Si@Mo JLs are the best candidate for H adsorption processes over pristine, Si@S and Si@Se JLs.