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Adsorption of monovalent aluminum halides on graphene defects
SUFIAN ALNEMRAT, JOSEPH HOOPER, Naval Postgraduate School — Density functional theory is used to study the adsorption of the monovalent aluminum halide AlCl on pristine and defective graphene (GR). Recent experimental efforts have shown that monovalent aluminum halide solutions can nucleate and grow small Al nanoparticles on a graphene surface. This nucleation and growth process may also shed light on how similar monovalent AlCl and AlBr solutions assemble into ligand-stabilized metalloid clusters. In this study we examined several point-type defects on GR to determine favorable sites for cluster nucleation. We found that the AlCl weakly physisorbs on pure GR, Stone-Wales point defects, and N-, B- doped-GR. On the other hand, the AlCl monomer chemisorbs on monovacancies, divacancies, and pyridine-like N, B, and O doped monovacancies. The binding energy is on the order of 5.0 eV and a strong covalent bond between the Al and the dangling bonds on the C-atoms near the defect sites is observed. In the pyridinelike N- and O-monovacancy defects, additional bonding between Al and the dopant-atoms results in the strongest binding energy of any graphene variant considered.

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