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First-principles study of interaction of silicene with amino acid analogues in solvated phase YESUKHEI JAGVARAL, HAIYING HE, Valparaiso Univ, RAVINDRA PANDEY, Michigan Tech. Uni — We have investigated the nature of adsorption of amino-acid analogues on silicene employing density functional theory and an implicit solvation model. Amino acid analogues are defined as CH3–R molecules, where R is the functional group of the amino acid side chain. We have found from the calculated results three distinct groups within the amino-acid analogues considered: (i) group I, which includes MeCH3 and MeSH, interacts with silicene via the van der Waals dispersive terms leading to physisorbed configurations; (ii) group II strongly interacts with silicene forming Si–O/N chemical bonds in the chemisorbed configurations; and (iii) group III, which consists of the phenyl group, interacts with silicene via π–π interactions leading to physisorbed configurations. The results show that the lateral chains of the amino acids intrinsically determine the interactions between protein and silicene at the interface under the given physiological conditions.

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