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Binding of solvated peptide (EPLQLKM) with a graphene sheet: all-atom-to-all residue hierarchical approach[1] AERIAL CAMDEN, ZHIFENG KUANG, RAJIV BERRY, RAJESH NAIK, BARRY FARMER, Air Force Research Laboratory, NADIA DRAGNEVA, WELY FLORIANO, OLEG RUBEL, Lakehead University, Canada, RAS PANDEY, University of Southern Mississippi — Binding of peptide EPLQLKM with a graphene sheet is studied by a coarse-grained computer simulation involving all-atom-to-all-residue interactions between amino acids and substrate. Estimates of the binding energy of amino acids with the graphene sheet in presence of aqueous solvent with three independent all-atom MD simulations are used as input to residue-substrate interaction in an all-residue coarse-grained representation of peptides. Large-scale Monte Carlo simulations are performed to examine the binding of peptides with the input of three simulation residue-substrate interactions as a function of temperature. Despite a considerable difference in quantitative estimates of the binding energy of amino acids with three all-atom simulations, the results of peptide binding, i.e., relative strength of binding (including anchoring residues) response to temperature remains the same. Differences and similarities in binding as a result of three simulated-interactions will be discussed in detail.

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