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A hierarchical coarse-grained (all-atom to all residue) approach to peptides (P1, P2) binding with a graphene sheet[1] RAS PANDEY, University of Southern Mississippi, ZHIFENG KUANG, BARRY FARMER, SANG KIM, RAJESH NAIK, Air Force Research Laboratory — Recently, Kim et al. [1] have found that peptides P1: HSSYWYAFNNKT and P2: EPLQLKM bind selectively to graphene surfaces and edges respectively which are critical in modulating both the mechanical as well as electronic transport properties of graphene. Such distinctions in binding sites (edge versus surface) observed in electron micrographs were verified by computer simulation by an all-atomic model that captures the pi-pi bonding. We propose a hierarchical approach that involves input from the all-atom Molecular Dynamics (MD) study (with atomistic detail) into a coarse-grained Monte Carlo simulation to extend this study further to a larger scale. The binding energy of a free amino acid with the graphene sheet from all-atom simulation is used in the interaction parameter for the coarse-grained approach. Peptide chain executes its stochastic motion with the Metropolis algorithm. We investigate a number of local and global physical quantities and find that peptide P1 is likely to bind more strongly to graphene sheet than P2 and that it is anchored by three residues ^{4}Y^{5}W^{6}Y. [1] S.N. Kim et al J. Am. Chem. Soc. 133, 14480 (2011).

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