Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Peptides (P1, P2 and its mutations) binding with a graphene sheet: an all-atom to all-residue hierarchical coarse-grained approach[1] ZHIFENG KUANG, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — Binding of peptide P2 (EPLQLKM) [1] and its mutations (P2G, P2Q) to a graphene sheet are studied by a coarse-grained computer simulation. Our hierarchical coarse-grained approach involves all-atom MD simulation to assess the binding interaction of each residue with the graphene sheet. Data from all-atom simulations are then used as input to phenomenological interaction in a coarse-grained MC simulation [2]. Binding of each peptide and its residue in corresponding sequence (P2, P2G, P2Q) are evaluated by analyzing the adsorption of each residue, its mobility, and structural profiles. Although it is difficult to identify overall morphological differences in adsorbed peptides by visual inspections, quantitative analysis of the conformational changes of adsorbed peptides shows variations in size among P2E and its mutations. Results on binding of peptide P1 (HSSYWYAFNNKT) may also be presented if data become available.

[1]This work is supported by the Air Force Research Laboratory.

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Date submitted: 02 Nov 2012 Electronic form version 1.4