Supplement

Stability of peptide (P1, P2) binding to a graphene sheet via an all-atom to all-residue coarse-grained approach

R.B. Pandey,[1] Zhifeng Kuang,[2] B.L. Farmer,[2] Sang N. Kim,[2] Rajesh R. Naik[2]

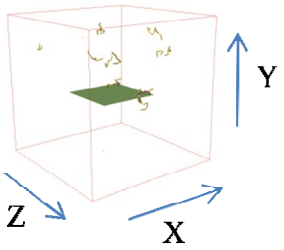

Figure S1: Graphene sheet (zx-plane) in presence of peptides to illustrate the orientations.

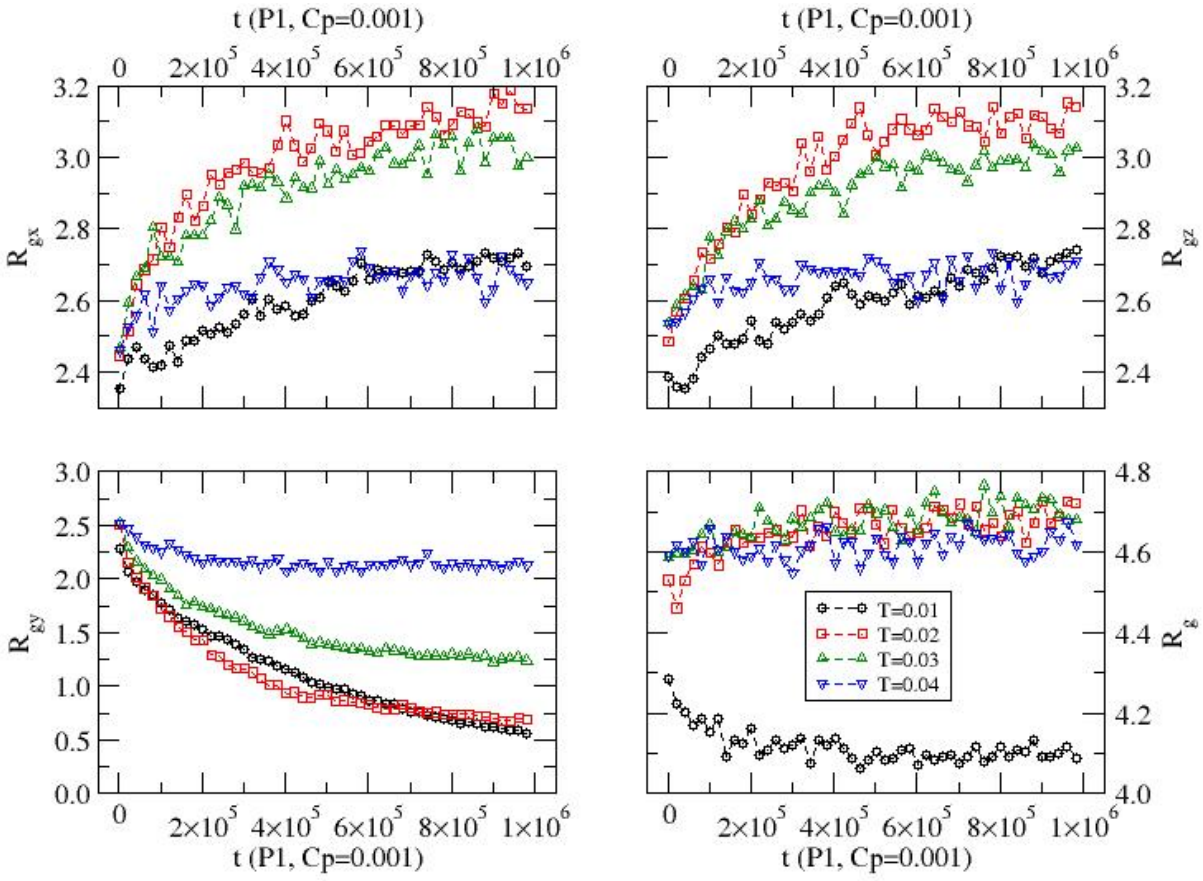

Figure S2: Variations of the average radius of gyration (R_g) (and its components (R_{gx}, R_{gy}, R_{gz})) of peptides P1 with the time steps at *T=0.01-0.04, Cp=0.001*. Simulations are performed on a 100^3 lattice with *100* independent samples.

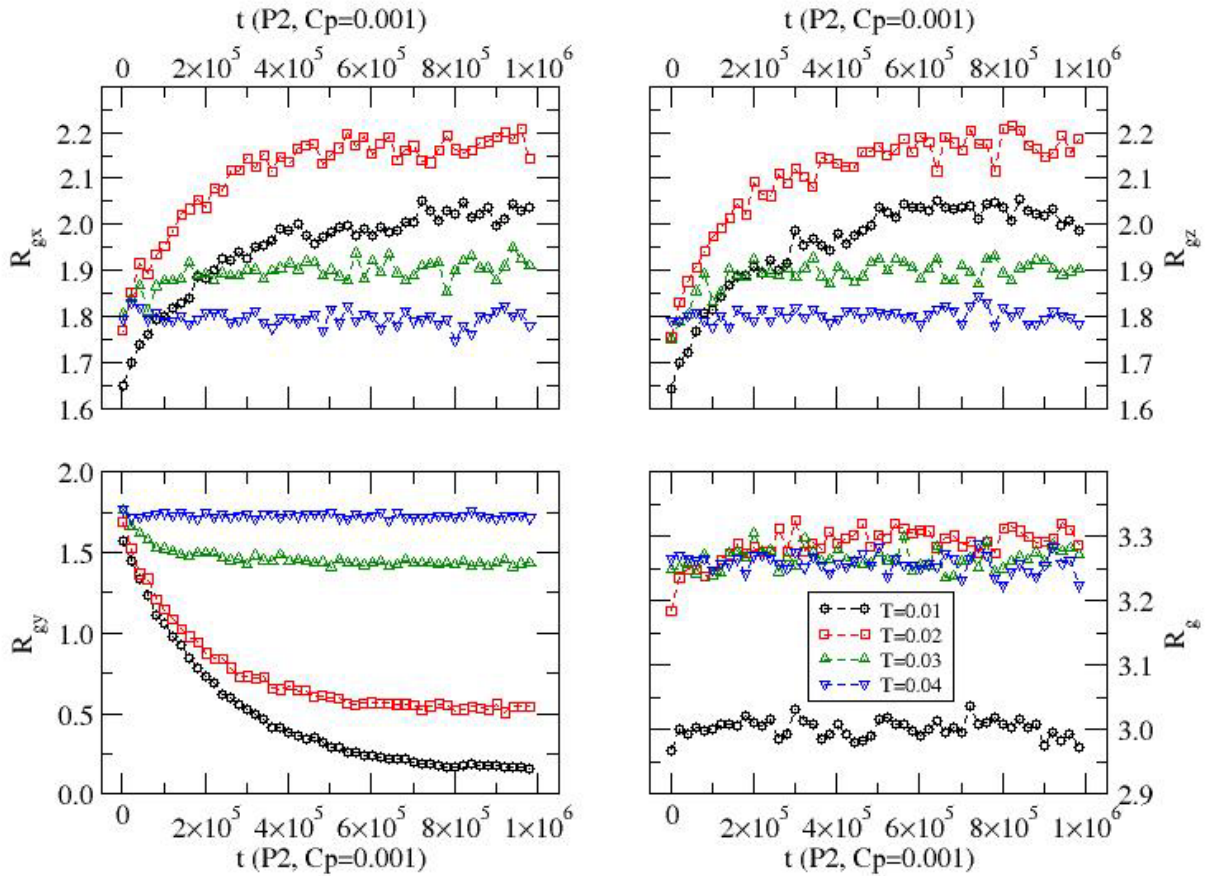

Figure S3: Variations of the average radius of gyration (R_g) (and its components (R_{gx}, R_{gy}, R_{gz})) of peptides P2 with the time steps at *T=0.01-0.04, Cp=0.001*. Simulations are performed on a 100^3 lattice with*100* independent samples.