Salinity, solvent, and oxidation degree of graphene on silica-graphene interactions

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We were interested in evaluating the effects of salinity, solvent, and the degree of graphene oxidation on the force required to detach graphene at α-silica (surface) using molecular dynamics. For this purpose, graphene with O/C ratios of 0, 0.2 and 0.4, salinities of 3000 and 30000 ppm NaCl, and water and toluene solvents in contact with α-silica were evaluated. All systems were sequentially stabilised in 3 ns of NVT, 3 ns NPT and 3 ns of NVT ensembles. Then, Steered method [1] with a spring constant of 138.96 pN/Å and a velocity of $2.4*10^{-5}$ Å*fs^{-1} was applied during 3.0 ns in an NVT ensemble at 298.15 K and 1.0 atm.

Our results showed that the degree of oxidation of graphene has effects on the interactions with in contact with α-silica surface. As shown in Figure 1a, the maximum force applied to detach graphene from the surface was highest for O/C ratio = 0 (approx. 3.5 nN), followed by O/C ratio = 0.2 (approx. 3 nN) and O/C ratio = 0.4 (approx. 2 nN). In addition, the solvent also showed effects on the interactions between the surface and graphene, as the maximum force to detach graphene from the surface decreased by approximately 1 nN when toluene was used as a solvent instead of water (Figure 1b). Nevertheless, salinity has no significant effect on the graphene-surface interaction.

Figures

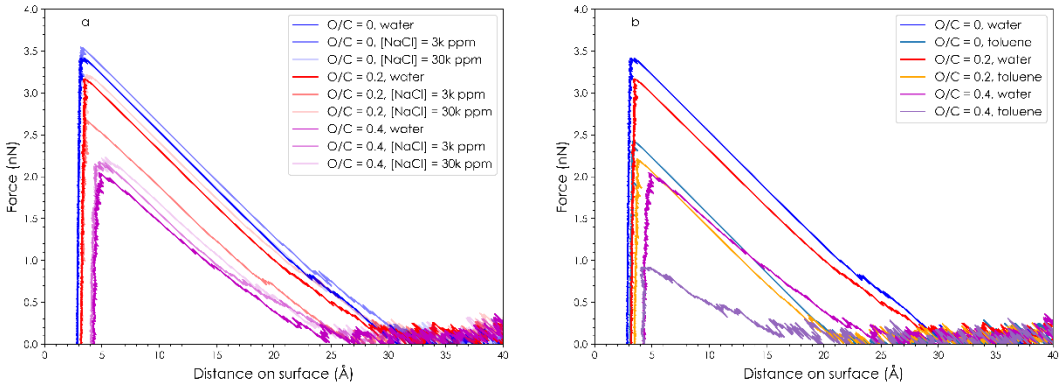

Figure 1: Salinity, solvent, and oxidation degree of graphene on silica-graphene interactions.

References

[1] S. Izrailev, S. Stepaniants, B. Isralewitz, D. Kosztin, H. Lu, F. Molnar, W. Wriggers, and K. Schulten, "Steered Molecular Dynamics" In P. Deuflhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, and R. D. Skeel, editors, Computational Molecular Dynamics: Challenges, Methods, Ideas, volume 4 of Lecture Notes in Computational Science and Engineering, pp. 39-65. Springer-Verlag, Berlin, 1998