Abstract Submitted
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Density Functional Theory and MD Simulations of Properties of PDMS near Silica Surfaces[1] SHYAMAL K. NATH, NM Institute of Mining & Technology, AMALIE L. FRISCHKNECHT, JOHN G. CURRO, Sandia National Laboratories, JOHN D. MCCOY, NM Institute of Mining & Technology — Polydimethylsiloxane (PDMS) is a very important polymer for its application in the adhesives, sealants, coatings and biomedical industries. In this work, we study the properties of PDMS melts confined between silica surfaces. We used two different approaches: First, a density functional theory (DFT) that uses the structure of the homogeneous liquid as input; and, second, full-scale molecular dynamics simulations. We used a fully detailed, realistic model of PDMS within the united atom framework in both the DFT and simulation studies. In solving the DFT equations, the direct correlation functions were obtained from PRISM theory with attractions treated via the random-phase approximation. Separate scaling factors were employed for the PRISM and RPA parts of the direct correlation functions. Good agreement was observed between DFT and MD simulations for density profiles, stress profiles, and surface tensions. We also made direct connection to experimental results by estimating the forces on the silica surface from DFT.

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John G. Curro
Sandia National Laboratories

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