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Molecular Dynamics calculation of solid/liquid surface tension: a methodological study NICOLAS PINEAU, THIBAUD DREHER, LAURENT SOULARD, EMERIC BOURASSEAU, CEA DAM DIF, PATRICE MALFREYT, Universit Blaise Pascal, Clermont-Ferrand — The influence of polymer/molecular crystal interfaces on the mechanical properties of Polymer Binded Explosives under high strains is an open topic which can be explored through surface tension calculations. While such calculations are being performed for liquid/liquid and liquid/vapor interfaces intensively (A. Ghoufi et al., Chem. Soc. Rev. 45 (2016), 1387), little is known for the solid/liquid and solid/solid interfaces. The aim of this work is to fill that gap by computing the solid/liquid surface tension of a simple model system consisting of a graphene sheet embedded in liquid methane. We show that, unlike the liquid/vapour and liquid/liquid systems, the presence of a solid substrate has a strong impact on the structure of the fluid phase and that the simulation parameters should be chosen carefully to compute accurate surface tensions.

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