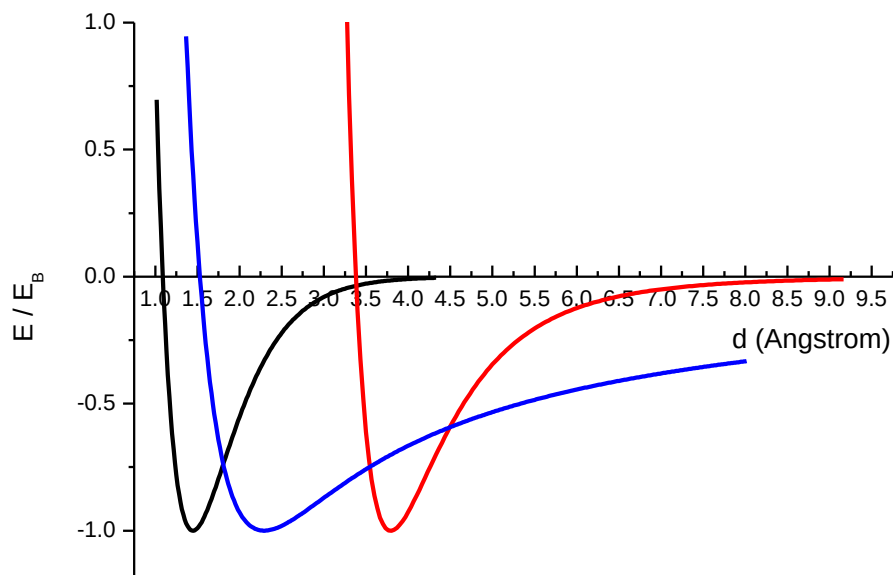


Übungsblatt 1

zur Abgabe am 30.10.2017

1) The graph below shows model potentials for the Ar_2 molecules, a C-C bond, and a NaCl molecule. Identify the respective potential curves. Discuss the differences in shape of the potential curves, in particular in the attractive part. Explain the nature of interactions which are reflected in these shapes.



2) Write up a potential for the interaction between carbon atoms in graphene by combining a Tersoff potential with an angular term as in the Stillinger-Weber potential. Assume that graphene is constricted to two dimensions. The bond order of carbon-carbon bonds in graphene is 1.33. Please explain in a few sentences your choice of potential and parameters.