Ab initio molecular dynamics simulation of hydrogen fluoride at several thermodynamic states

Liquid hydrogen fluoride is a simple but interesting system for studies of the influence of hydrogen bonds on physical properties. We have performed ab initio molecular dynamics simulations of HF at several thermodynamic states, where we examine the microscopic structure of the liquid as well as its static and dynamic properties. The results obtained show good agreement with well established data, and, moreover, we were able to show significant changes within the structure depending on the system's temperature and density.

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