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

**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.

**General information**
Publication status: Published
Organisations: Department of Physics, University of Stuttgart, Hoenggerberg HCI
Contributors: Kreitmeir, M., Bertagnolli, H., Mortensen, J. J., Parrinello, M.
Pages: 3639-3645
Publication date: 2003
Peer-reviewed: Yes

**Publication information**
Journal: Journal of Chemical Physics
Volume: 118
Issue number: 8
ISSN (Print): 0021-9606
Ratings:
Scopus rating (2003): SJR 2.275 SNIP 1.375
Web of Science (2003): Indexed yes
Original language: English
Keywords: SYSTEMS, HF, LIQUID WATER, SCATTERING, WANNIER FUNCTIONS, COMPUTER-SIMULATION, DENSITY, DEUTERIUM FLUORIDE
Electronic versions:
Markus.pdf
DOIs:
10.1063/1.1539045
URLs:
http://link.aip.org/link/JCPSA6/v118/i8/p3639/s1

**Bibliographical note**
Copyright (2003) American Institute of Physics. This article may be downloaded for personal use only. Any other use requires prior permission of the author and the American Institute of Physics.
Source: orbit
Source ID: 23096
Research output: Contribution to journal › Journal article – Annual report year: 2003 › Research › peer-review