



Periodic Hartree-Fock study of $(\text{HF})_\infty$ chain.

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Streszczenie

The periodic Hartree-Fock study has been performed for the hydrogen fluoride chain. Double and triple zeta basis sets were used for calculation of structural and electronic properties. The large effect of standard sp diffuse functions was observed on the band structures and density of state. The polarisation functions and basis set of triple-zeta quality seem to be less important for description of electronic properties. For structural considerations 6-31G(d,p) basis set should be applied though it gives too short length of the F-H bond.

Słowa kluczowe

Ab initio, Band structure, Diffuse function, Hydrogen fluoride chain, Periodic Hartree-Fock

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