DFT study of octanuclear molecular chromium-based ring using new pseudopotential parameters

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Molecular magnets play very important role in fundamental physics since these systems have shown new magnetic and electronic futures and revealed to be promising for possible applications in quantum computing and magnetoelectronics. Among these systems, there are homonuclear antiferromagnetic ring-shaped molecules formed by transition metal ions in an almost planar ring.

9.7 cm

We present a comprehensive study of electronic and magnetic properties of $Cr_8F_8Piv_{16}$ molecular ring (in short Cr8) using the package SIESTA with several choices of chromium pseudopotential parameters. We use generalized gradient approximation (GGA) to investigate properties of Cr8 ring approximated by replacing the pivallic group by H atoms (hydrogen saturation). For different choice of chromium pseudopotential we examine the electronic and magnetic properties of Cr8 molecule. We compare the density of states, electron density maps and HOMO-LUMO energies. Also magnetic properties are studied in detail - magnetic moments and exchange interaction parameter J are presented. The influence of pseudopotential parameters on obtained results is discussed. Finally our results are compared with other theoretical approaches and experimental data.

13.4 cm

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