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Spin density functional study on magnetism of potassium-loaded Zeolite A YOSHIRO NOHARA, University of Tokyo, KAZUMA NAKAMURA, RYOTARO ARITA — In order to clarify the mechanism of spin polarization in potassium-loaded zeolite A, we perform *ab initio* density-functional calculations. We find that (i) the system comprising only non-magnetic elements (Al, Si, O and K) can indeed exhibit ferromagnetism, (ii) the host cage makes a confining quantum-well potential in which superatom s- and p-like states are formed, the latter p states are responsible for the spin polarization, and (iii) the size of the magnetic moment depends sensitively on atomic positions of potassium clusters. We show that the spin polarization can be described systematically in terms of the confining potential and the crystal-field splitting in the superatom p states. (arXiv 0909.4432 (2009))

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