

***Ab-initio* study of IFR zeolite with Cs atoms within the channels**

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We report self-consistent *ab-initio* calculations of structural and electronic properties for a kind of recently synthesized inorganic electrides. The optimized geometry gives zigzag Cs atoms chains within the sinusoidal channels of the zeolite. And we find that a finite density of states appears at the Fermi level by our electronic structure calculations. Among the wide gap of the zeolite, near the conduct bands, there are four bands mainly contributed from 6s electrons of Cs atoms, which have a delocalized real space distribution along the channels. The shift of Fermi level and the delocalization of the highest occupied band make this material a powerful reducing agent.