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Theoretical Study of Encapsulated Alkali Metal Atoms in Nanoporous Channels of ITQ-4 Zeolite: One-Dimensional Metals and Inorganic Electrides[1] HONG LI, S. D. MAHANTI, Department of Physics and Astronomy, Michigan State University — Electronic structure calculations within density functional theory have been carried out in a class of *M*-ITQ-4 zeolite (*M* = Na, K, Rb, Cs) to understand the competing effects of guest-guest (*M*-*M*) and guest-host (*M*-ITQ-4) interactions. These compounds are known as inorganic electrides because the state of the valence electron of the alkali atom is manipulated by trapping the alkali atoms inside inorganic zeolite channels [1,2]. We find that the arrangements of alkali atoms in the ITQ-4 zeolite channel change dramatically in going from Cs to Na. In Na-ITQ-4, the Na atoms form a nearly perfect 1D metal undergoing Peierls distortion and concomitant dimerization. However, in Cs-ITQ-4, the Cs atoms form a zig-zag chain and couple rather strongly to the host. The calculated geometry for Cs-ITQ-4 zeolite is in very good agreement with the pair distribution function (PDF) measurement [3]. Optical absorptions have also been calculated which are in qualitative agreement with experiment. In addition to the guest-host high energy excitations ranging from 0.54 eV to 2.10 eV, we also find an infrared peak at 3300 nm, which should be carefully tested by experiments.

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3. V. Petkov *et. al.*, Phys. Rev. Lett. **89**, 075502 (2002).

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