Theoretical Study of Encapsulated Alkali Metal Atoms in Nanoporous Channels of ITQ-4 Zeolite: One-Dimensional Metals and Inorganic Electrides\textsuperscript{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 ($M = \text{Na, K, Rb, Cs}$) 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\textsuperscript{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\textsuperscript{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.


\textsuperscript{1}Supported by National Science Foundation through Grant No. CHE0211029 and Michigan State University.

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Date submitted: 07 Dec 2004

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