Optical properties of guest Na- and Rb-atoms in quasi-2D $M_{7.8}Al_{7.8}Si_{8.2}O_{32.0}$ (M = Na, Rb) from the perspective of polarons in a deformable lattice

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Introduction

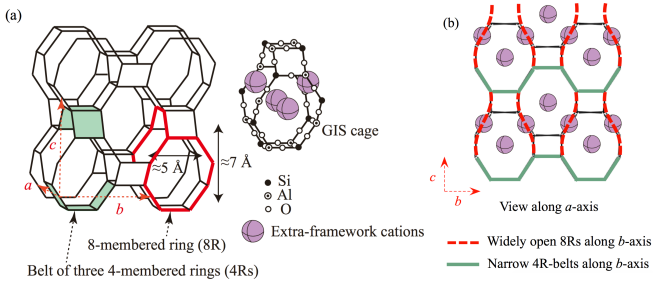
Electron-phonon interaction plays an important role in strongly-correlated electron systems. Optical and related electronic properties can be fine-tuned by adjusting the deformation potential felt by electrons in a system, and remains a less explored avenue.

Aim

Explore the possibility to fine-tune optical excitations of electrons making use of a deformable lattice that leads to local lattice distortions and symmetry-breaking due to electron-phonon interactions.

Materials and Methods

A quasi-two-dimensional framework ($Al_{7.8}Si_{8.2}O_{32.0}$) is used to confine electrons in nearly-two-dimensional space. The framework contains a deformable lattice made-up of displaceable cations ($M_{7.8}$).



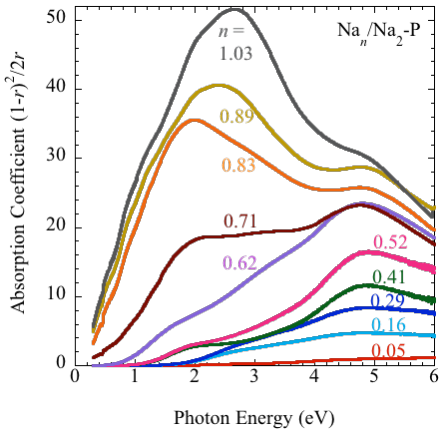
Optical properties are investigated making use of diffuse reflectance of powder particles and Kubelka-Munk transformations to obtain optical absorption.

Results

$M_{7.8}Al_{7.8}Si_{8.2}O_{32.0}$: Four cages, Na_2-P: Abbreviation for one-cage, n: Guest atoms per cage

Guest Na atoms in $Na_{7.8}Al_{7.8}Si_{8.2}O_{32.0}$

Broader absorptions

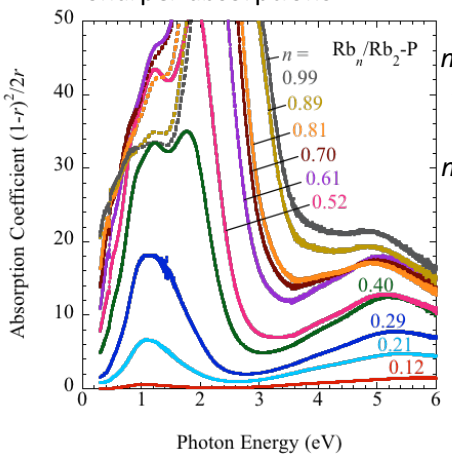


$n < 0.4$
2.5 and 4.8 eV

$n > 0.4$
2.0 and 4.8 eV

Guest Rb atoms in $Rb_{7.8}Al_{7.8}Si_{8.2}O_{32.0}$

Sharper absorptions

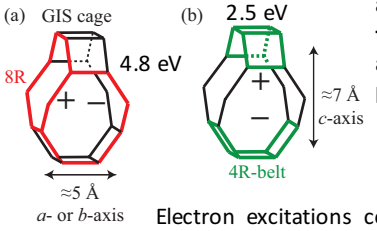


$n < 0.4$
1.1 eV

$n \geq 0.4$
1.1 and 2 eV

2 eV peak shifts to higher energy

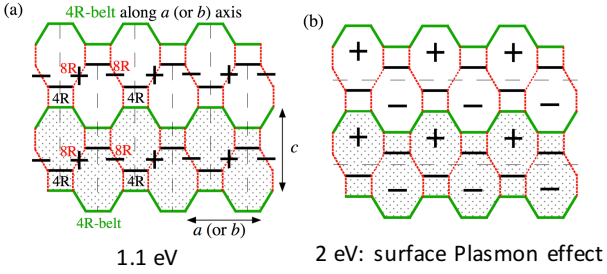
Discussions



Electron excitations confined in a cage

Strong electron-phonon interaction of Na cations and 3*s* electron leading to larger deformations and strong electron localization

Lesser effect of electron-phonon interaction



1.1 eV

2 eV: surface Plasmon effect

Electron excitations in two-dimensional channels

Electron-phonon interaction (polarons) strongly modifies the optical properties
Further experimental and theoretical investigations of the polaron effect are needed