

THE ELECTRONIC STRUCTURE AND SPECTRAL CHARACTERISTICS OF $\text{Na}_8\text{Si}_{46}$, $\text{Ba}_8\text{Si}_{46}$ CLATHRATES AND HYPOTHETICAL $\text{Mo}_8\text{Si}_{46}$ CLATHRATE

Borsch N. A., Pereslavl'tseva N. S., Kurganskii S. I.

In this work the results of electronic structure calculations of $\text{Na}_8\text{Si}_{46}$, $\text{Ba}_8\text{Si}_{46}$ clathrates and hypothetical $\text{Mo}_8\text{Si}_{46}$ clathrate are presented. In calculation the linearized augmented plane wave method was used. Band structure, total and partial density of states and x-ray emission Si $K_{\beta 1,3,-}$ and Si $L_{2,3,-}$ spectra was obtained as results of calculation. The comparison of calculated and experimental spectra for $\text{Na}_8\text{Si}_{46}$ are presented.