

CHEMISTRY

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How to Derive a Meaningful Bonding Model for CuAl_2 -type Intermetallic Compounds?

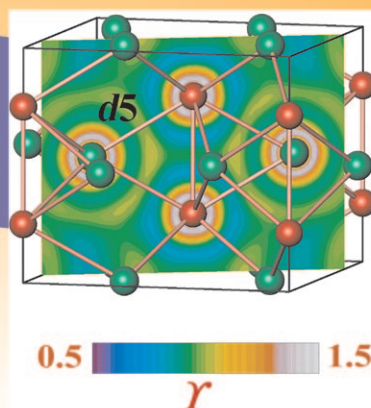
Structural Data

Space group $I4/mcm$

Pearson Symbol $tI12$

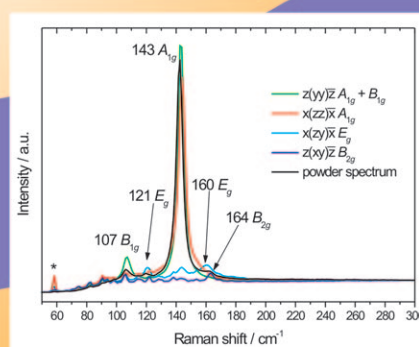
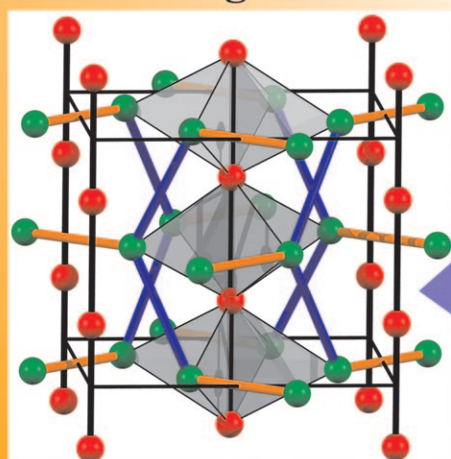
A $4a$ (0 0 $\frac{1}{4}$)

B $8h$ (x x 0)



Quantum Chemistry

Bonding Model



Physical Properties

The description of the chemical bonding...

... in intermetallic compounds is often not straight forward. Based on the electron localization approach the chemical bonding in intermetallic compounds is described in real space by M. Armbrüster et al. in the Full Paper on page 10357 ff. Physical property measurements were applied to verify and quantify the chemical bonding model, resulting in a physically meaningful description of the chemical bonding situation for intermetallic compounds with the CuAl_2 type of structure.



Inside Cover

Marc Armbrüster*, Walter Schnelle, Raul Cardoso-Gil, and Yuri Grin

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