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Data Article

Data from the electronic band structures of several Zintl phases with group 15 elements and the transition metals

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ABSTRACT

Electronic band structures of the following compounds – $Cs_4Cd(As_7)_2$, K_2PdP_2, K_5CuAs_2, Na_2CuP and $K_3Cu_3P_2$ – all computed by means of the TB-LMTO-ASA code. The calculations show that for all compounds, the bonding states are occupied, while the anti-bonding orbitals are vacant. This confirms the partitioning of the valence electrons according to the Zintl–Klemm formalism. *The data is related to* doi.org/10.1016/j.jssc.2018.11.029 (Ovchinnikov and Bobev, 2019) [1].

Specifications table

Subject area	*Chemistry, materials science*
More specific subject area	*Solid-state chemistry*
Type of data	*Graph, figure*
How data was acquired	*Calculations on the electronic band structure via the TB-LMTO code.*
Data format	*Analyzed*
Experimental factors	In the figures, the electronic density of states (DOS) is given in states eV^{-1} (primitive unit cell)$^{-1}$.

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Experimental features	*Bonding is optimized in all structures, i.e., all bonding orbitals are occupied and all antibonding orbitals are vacant, the ground state of a Zintl phase has an energy gap between the valence and conduction bands, resulting in semiconducting behavior.*
Data source location	*University of Delaware, Newark DE 19716, U.S.A.*
Data accessibility	*Data is with this article*
Related research article	*"Zintl Phases with Group 15 Elements and the Transition Metals: A Brief Overview of Pnictides with Diverse and Complex Structures" Alexander Ovchinnikov and Svilen Bobev, Journal of Solid State Chemistry,* doi.org/10.1016/j.jssc.2018.11.029 [1].

Value of the data

- The data from all computed band structures show small-to-medium sized energy bandgaps, as expected from the rationalization of the crystal structures.
- The data from all computed band structures can be used to show that the transition metal states are partially filled.
- The data confirms that all studied compounds have optimal number of valence electrons.

1. Data

The graphs for the projected total and partial density of states for $Cs_4Cd(As_7)_2$ (Fig. 1), K_2PdP_2 (Fig. 2), K_5CuAs_2 (Fig. 3), Na_2CuP (Fig. 4), and $K_3Cu_3P_2$ (Fig. 5) all show electronically gapped ground states, in line with the classification of the title compounds as Zintl phases.

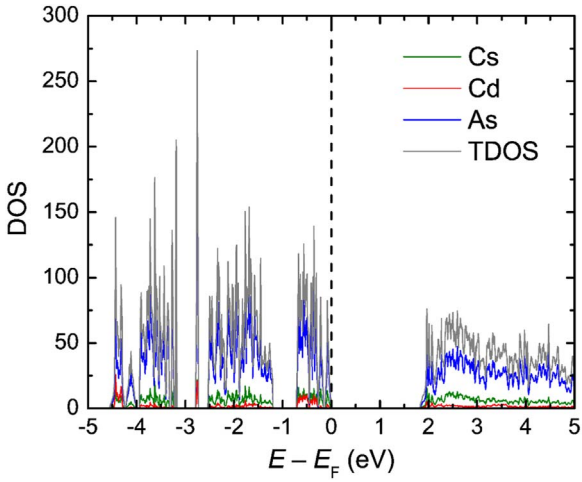

Fig. 1. Total and projected DOS for $Cs_4Cd(As_7)_2$, space group $P2_1/c$, Pearson symbol $mP76$.

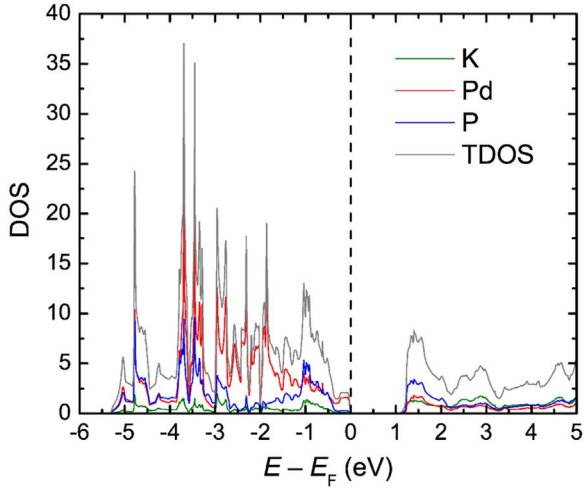

Fig. 2. Total and projected DOS for K_2PdP_2, space group *Cmcm*, Pearson symbol *oS*20.

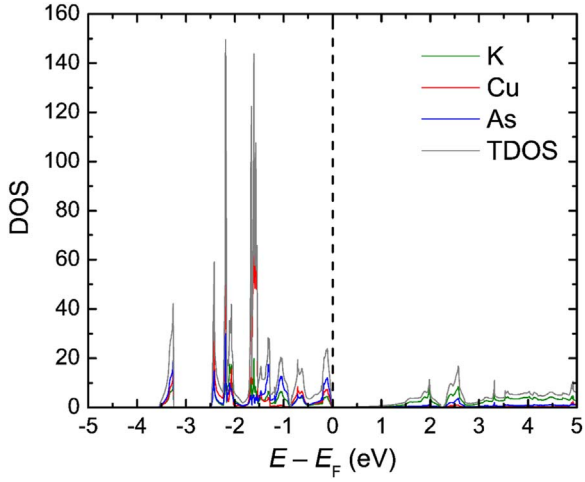

Fig. 3. Total and projected DOS for K_5CuAs_2, space group $P6_3/mmc$, Pearson symbol *hP*16.

2. Experimental design, materials, and methods

The first-principle calculations presented here were done using the TB-LMTO-ASA code [2] with the von Barth–Hedin implementation of the local density approximation (LDA) functional [3]. To satisfy the atomic sphere approximation (ASA), empty spheres were generated by the automatic procedure within the LMTO code [2]. Chemical bonding was analyzed with the aid of Crystal Orbital Hamilton Population curves (COHP). Atomic parameters from the experimental crystal structures were used. In the provided diagrams, the electronic density of states (DOS) is given in states eV^{-1} (primitive unit cell)$^{-1}$. Fermi level is set as a reference point at 0 eV.

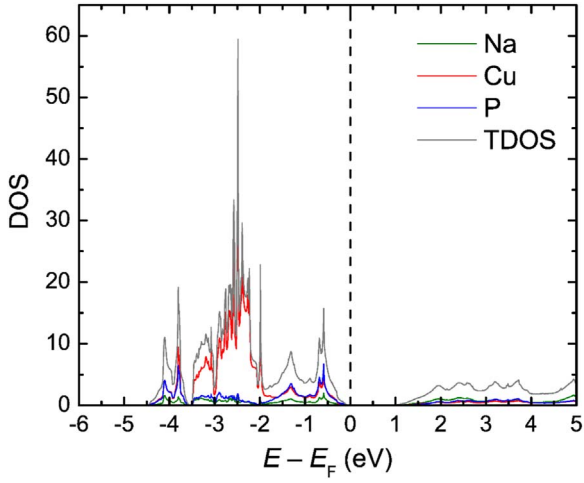

Fig. 4. Total and projected DOS of Na_2CuP, space group *Cmcm*, Pearson symbol *oS*16.

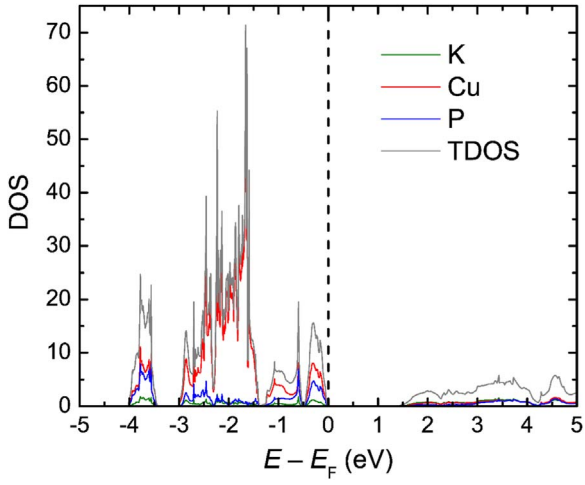

Fig. 5. Total and projected DOS for $K_3Cu_3P_2$, space group $R\bar{3}m$, Pearson symbol *hR*8.

Acknowledgments

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Transparency document. Supplementary material

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.12.040.

References

[1] A. Ovchinnikov, S. Bobev, J. Solid State Chem. 270 (2019) 346–359. https://doi.org/10.1016/j.jssc.2018.11.029.
[2] O. Jepsen, O.K. Andersen, The Stuttgart TB-LMTO-ASA Program, Version 4.7, Max-Planck-Institut Für Festkörperforschung, Stuttgart, Germany, 1999.
[3] U. von Barth, L. Hedin, J. Phys. C Solid State Phys. 5 (1972) 1629–1642.