

# The all-electron APW code WIEN2k: Applications to phonon related properties

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I will give a review on augmented plane wave (APW) methods for the calculation of the electronic structure in solids starting with the original concept developed by J. Slater [1] long time ago up to the APW+lo method introduced by Sjöstedt *et al.* [2]. This latter method combines the superior convergence behaviour of the original APW method with the convenience of LAPW [3]. I will then give an overview of the implementation of APW+lo into the WIEN2k code [4] and summarize the available features and discuss in particular the possibilities connected with calculations of phonons.

Selected results will be discussed in more detail. This will include phase transitions in  $\text{RbCaF}_3$  [5] and  $\text{PbTiO}_3$  [6] as well as a finite temperature (phonon) related explanation of a double peak occurring in the B-K XANES spectra of h-BN [7].

## Refs

- [1] J. Slater, Phys. Rev. **51**, 151 (1937).
- [2] E. Sjöstedt, L. Nordström and D. Singh, Solid State Commun. **114**, 15 (2000).
- [3] G. K. H. Madsen, P. Blaha, K. Schwarz, E. Sjöstedt and L. Nordström, Phys. Rev. B **64**, 195134 (2001).
- [4] <http://www.wien2k.at>
- [5] S. Ehsan, A. Tröster, F. Tran and P. Blaha, Phys Rev. Mat. **2**, 093610 (2018).
- [6] A. Tröster, S. Ehsan, K. Belbase, P. Blaha, J. Kreisel and W. Schranz, Phys. Rev. B **95**, 064111 (2017).
- [7] F. Karsai, M. Humer, E. Flage-Larsen, P. Blaha and G. Kresse, Phys. Rev. B **98**, 235205 (2018).

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