Some numerical methods for electronic structure calculations in solids

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Abstract: In this talk, I will first present an algorithm to construct composite Wannier functions for $2D$ and $3D$ periodic crystals with time-reversal symmetry, based on ideas from [2] and [3].

This algorithm is more robust than the Marzari-Vanderbilt algorithm initialized with the projection method, since it cannot get trapped in 'false local minima' [4]. This is a joint work with A. Levitt, G. Panati and G. Stoltz [1].

If time allows, I will also briefly present some results obtained in collaboration with Y. Maday and co-workers related to our long-term research program on error analysis for first-principle simulation methods.

[1] E. Cancès, A. Levitt, G. Panati and G. Stoltz, *Robust determination of maximally-localized Wannier functions*, in preparation.
[2] H. Cornean, I. Herbst, and G. Nenciu, *On the construction of composite Wannier functions*, Ann. Henri Poincaré, in press.
[3] D. Fiorenza, D. Monaco, and G. Panati, *Construction of real-valued localized composite Wannier functions for insulators*, Ann. Henri Poincaré, 17(1):63–97, 2016.
[4] N. Marzari and D. Vanderbilt, *Maximally localized generalized Wannier functions for composite energy bands*, Phys. Rev. B, 56(20):12847, 1997.