# Wannier functions: from topology to polarization and magnetization


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Wannier functions are localized wave functions that can be used to build up arbitrary wave packets travelling through a crystal. They are not electron energy eigenfunctions themselves, but are superpositions of those energy eigenfunctions. In recent years it has been shown under what circumstances such functions can be built that are "exponentially localized" – that is, that are very confined to the neighborhood of a particular unit cell. One of the most important recent developments in condensed matter physics is the demonstration of how these "exponentially localized Wannier functions" (ELWFs) are connected to the topology of the underlying band structure of the crystal, and not just to its spectral properties. And these ELWFs are central to a modern, quantum mechanical description of the polarization and magnetization fields that you learned about in your second year course in electromagnetic theory.

After an introduction to the physics of these matters, the project will involve numerical and analytical studies of these Wannier functions and how they can be used to help describe the properties of crystals, particularly their optical properties. Some of the numerical work will be done using part of the *OpenMX* suite of codes (http://www.openmx-square.org/whatisopenmx.html), and others, to calculate the Wannier functions, which will then be used to address various crystal properties. Initial familiarity with these codes is not essential, but familiarity with Python and a good grasp of quantum mechanics at least at the third-year level is essential. The project is suitable for students who have completed at least their 3rd year of undergraduate study.