“Wannier functions: Visualizing chemistry in crystalline solids”

In solid state physics, the usual description of the occupied states is in terms of Bloch states, which are wave-like states that extend throughout the entire crystal. However, for many purposes a description in terms of local chemistry is more useful. In this spirit, Boys and others developed “localized molecular orbitals” for molecular systems, and the corresponding objects in crystals go under the name of “Wannier functions.” In recent years, methods based on the construction and use of Wannier functions have gained traction in the theoretical electronic structure community. I will explain what Wannier functions are, discuss how they facilitate studies of chemical bonding in crystals, and survey some of their many uses. For example, Wannier-based methods can be used to investigate dielectric and transport properties, perform high-quality interpolation of band structures, and identify topological materials.

David Vanderbilt received his BA in Physics from Swarthmore College in 1976 and his PhD in Physics from the Massachusetts Institute of Technology in 1981. He spent three years as a Miller Postdoctoral Fellow at the University of California at Berkeley before joining the faculty of the Physics Department at Harvard University in 1984, first as an Assistant and then as an Associate Professor. He has been a Professor in the Department of Physics and Astronomy at Rutgers University since 1991, and was named Board of Governors Professor of Physics in 2009. Dr. Vanderbilt is an expert in the development of methods for electronic structure calculations and the application of such methods for computational materials theory. His current research interests include the development of methods for treating insulators in finite electric fields, advancing the theory and applicability of Wannier functions, and applying Berry-phase methods to study magnetic systems. One class of applications focuses on the dielectric and piezoelectric properties of novel oxide materials, especially structural phase transitions, lattice contributions to dielectric and piezoelectric activity, and properties of interfaces and superlattices. Another research thrust is concerned with anomalous Hall conductivity, orbital magnetization, magnetoelectric couplings, and topological insulators. Dr. Vanderbilt has published over 300 articles in scientific journals and has a Web of Science h-index of 90. He became a Fellow of the American Physical Society (APS) in 1995, is a winner of the 2006 Rahman Prize in Computational Physics awarded by the APS, and served as Chair of the Division of Materials Physics of the APS in 2006. He was awarded a Simons Fellowship in Theoretical Physics in 2014. He was elected to the National Academy of Sciences in 2013, and to the National Academy of Arts and Sciences in 2019.