Condensed Matter / Biophysics Seminar

Electronic structure of disordered solids

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Thursday

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4:00 P.M.

Rm 184 NSH

Understanding the physics of structurally disordered materials is a challenge to experimentalists and theorists alike. In this talk, I discuss the character of electronic states in disordered materials and emphasize the interplay between structure and electronic properties[1]. I begin by discussing the consequences of atomic structural disorder on electron states. As shown long ago by Anderson, disorder in atomic coordinates creates spatially confined or "localized" electron eigenstates near the Fermi level. I directly explore these states with large and realistic structural models and suitable electronic structure techniques. I begin with the structure of electron states in large and realistic models of a-Si, glassy silica and amorphous graphene, and find that important aspects of the states are universal (similar in different materials, and even for different physical quantities, such as classical vibrations). Next, we demonstrate the existence of subtle spatial correlations in the atomic coordinates (one-dimensional filaments or strings of connected long or short bonds) and show that these structures are responsible for the electronic band tails measured in photoemission and optical absorption experiments. We offer a partial solution to the "Urbach problem", explaining the experimental observation of exponential band tails in virtually all disordered systems[2]. The impact of the electronic structure on the atomic structure is discussed next, and I show that the electron states near the Fermi level determine the range of interatomic interactions, and thus play an important role in determining the structure itself[1]. The spatial decay of generalized Wannier functions[3] in these materials quantitatively measures the degree of non-locality of quantum mechanics in amorphous silicon (Fig. 1).

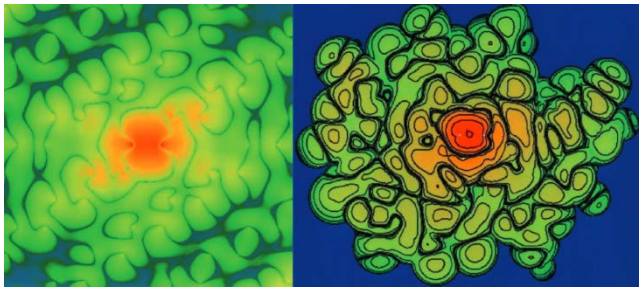

Fig. 1 Generalized Wannier function in diamond (left) and amorphous silicon (right).

1. D. A. Drabold, *Topics in the theory of amorphous materials*, European Physical Journal B **68** 1 (2009).
2. Y. Pan, F. Inam, M. Zhang and D. A. Drabold, *Atomistic origin of Urbach tails in amorphous silicon*, Phys. Rev. Lett. **100** 206403 (2008).
3. R. M. Martin, *Electronic Structure*, Cambridge University Press (2004). pp 469-470.