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Spin-Orbit Coupling, Strong Interactions, and Topological Character[1]

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In recent years the electronic structure of crystalline solids has come under close scrutiny because of the various types of topological characters that may arise. Most of the work is done at the one-electron (non-interacting) level, and most innovations have arisen from model tight-binding Hamiltonians and their eigenvectors. This talk will focus on a few examples of *discoveries made computationally* through DFT studies of actual materials, thus providing a physical realization as the discovery was made. Competition and partnership between strong interactions and spin-orbit coupling will be emphasized. Examples will include (1) the 'semi-Dirac' point Fermi surface phase in VO_2 thin films, the first member of a class now called *multi Weyl*: massive in some direction, massless in other direction; (2) a nodal loop semimetal phase found in computational studies of thin $SrVO_3$ films, realized more recently in NbP etc.; (3) the buckled honeycomb lattice of a (111) bilayer of $LaMnO_3$ encased on $LaAlO_3$, which is a Chern insulator and may be a realization of the Weyl-Mott insulator proposed recently by Morimoto and Nagaosa. Acknowledgments: R. Pentcheva, V. Pardo, K.-W. Lee, S. Gangopadhyay.

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