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Investigating Impurities on 3D Topological Insulators with Multiple Scattering Theory ROBERT VAN WESEP, University of Tennessee - Knoxville/Oak Ridge National Lab — Recently a new class of materials, three-dimensional topological insulators (3DTI), have generated significant theoretical and experimental interest due to surface states (SS) exhibiting linear dispersion at a Dirac point that are protected by time-reversal symmetry (TRS). Using magnetism to break TRS is of particular interest, especially via the deposition of magnetic impurities (MI) on the 3DTI surface. Experimental studies are in the early stages and consensus on the effect of MI on 3DTI SS has yet to be reached. Multiple scattering theory (MST) has proven useful in investigating surfaces, impurities and disordered systems and provides an ideal framework for first-principles, computational study. This presentation will report on progress in adapting MST to 3DTI systems with impurities.

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