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First-Principles Studies of TiAsRh, a new Dirac nodal line system SOPHIE WEBER, Department of Physics, UC Berkeley, RU CHEN, Lawrence Berkeley National Laboratory, QIMIN YAN, Temple University, Lawrence Berkeley National Laboratory, JEFFREY NEATON, Department of Physics, UC Berkeley; Molecular Foundry, LBNL — A recent development in condensed matter physics is the discovery of topological semimetals which have features in the band structure protected by an interplay of symmetry and topology. Dirac Nodal Line (DNL) systems are one such class of materials in which the conduction and valence bands touch in a closed loop in momentum space. Using density functional theory (DFT) calculations, we propose that TiAsRh is a DNL system and study the symmetry leading to the DNL. We find that a mirror plane protects the crossings without spin-orbit coupling (SOC), and demonstrate that SOC modestly gaps out the NL. We perform our study with standard semi-local and hybrid density functionals and show that the nodal line is robust with respect to functional. Implications for experiments on this compound, which has been previously synthesized, are discussed.

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