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Density Functional Theory studies of Epitaxial Charge Transfer Salts GEOFFREY A. ROJAS, P. GANESH, SIMON KELLY, BOBBY J. SUMPTER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JOHN A. SCHLUETER, Materials Science Division, Argonne National Laboratory, PETRO MAKSYMOVICH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Some of the fulvalene-based charge transfer salts (CTS) become superconducting in bulk. The basic physics and ways to control it has been explored by changing the intermolecular spacing using both chemical substitution and pressure, but the fixed stoichiometry limit the occupation of the filled states to what is naturally available. Recent experiments suggest growth of 2D epitaxial layers of CTS allowing stoichiometric and geometric control of the electronic structure, thereby leading to engineered superconducting interfaces. In a combined experiment and theory study, we provide new insight to understand the interplay between structure, stoichiometry and electronic-structure of epitaxially grown (ET)2SF5CH2CF2SO3 salt on Ag(111) surface. Density functional theory studies show that the cohesive energy of the 2D salts are very high, in spite of strong bonding to the underlying Ag surface via Ag-S metallic bonds, and provide a rationale for off-stoichiometric growth with different electronic structures as seen in our experiments, such as 3:1 and a 1:1 cation:anion stoichiometry, necessary for a monolayer coverage and different from the bulk 2:1 stoichiometry. We also explore the role of van der Waals interactions for structural stability. This research was conducted at the Center for Nanophase Materials Sciences, sponsored at ORNL by the Division of User Facilities, U.S. DOE.

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