

Evolution of electrider behaviour under pressure

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Electrides are a unique class of ionic materials in which the anions are stoichiometrically replaced by localised electrons. The localised electron gives electrider a number of unique properties including high hyperpolarisabilities, high magnetic susceptibilities, highly variable conductivities, extremely low work functions, low-temperature thermionic emissions and very strong reducing character. However, the majority of the known electrider are unstable at room temperature and consequently experimental studies of these materials are difficult. Theoretical modelling of these systems can greatly benefit the exploration of these materials.

We use density-functional theory (DFT) to show the presence of a localised electron and high lying "electrider" valence state in all of the known electrider. Pressure calculations are then conducted to explore the stability range of electrider under pressure. This helps identify ideal crystal void sizes and is the beginning of elucidating a directed design criteria for electrider.

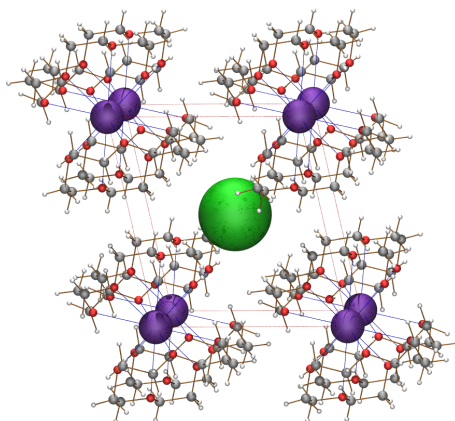


Figure 1: The crystal structure of Cs⁺(15-crown-5)₂e⁻, the simplest organic electrider, with a representative sphere placed at the approximate electron location.