Prediction of helium oxide molecule trapped in the electric field of two LiF dipoles

Elemental helium (He) is a prototypical noble gas and its atom sets the records many physicochemical properties. With its two electrons in the closed 1s shell, He is the smallest, the least polarizable, the most difficult to ionize, and the most electronegative atom known. Helium gas is considered to be as close to ‘ideal gas’ as possible and used as a standard of compressibility and pressure. Our subconscious perception of elemental helium is shaped by images of a colourless cryo-coolant, an ultra-cold and easy boiling-off liquid, which never freezes at ambient pressure but (rather costly!) disappears into a gas phase and once lost – inevitably leaves the gravitational field of planet Earth.

In consequence of its closed-shell electronic configuration, He also exhibits chemical inertness: non–charged molecules which contain chemically bound helium have not been synthesized to date. In the past theoreticians have tried to predict various neutral systems which contained chemically bound helium atom, but none held great promise; these species either exhibited very weak helium–element bonds at the limit of strong polarization interactions (He…BeO) or their estimated lifetime did not surpass nanosecond ($10^{-9}$ s) regime (HHeF).

In his research report Wojciech Grochala from the University of Warsaw (Poland) has now theoretically investigated a helium oxide molecule embedded inside a “ferroelectric cavity” composed of two parallel LiF molecular dipoles. Grochala was able to predict, using quantum mechanical methods, that this small neutral species, (HeO)(LiF)$_2$, should be planar with the polarized He$^{\delta+}$O$^{\delta-}$ unit. The calculations suggest that (HeO)(LiF)$_2$ is metastable: distortions which could disintegrate the molecule, can be suppressed at very low temperatures as all of the lowest vibrational levels sit in the local potential energy well.

Successful preparation of neutral (HeO)(LiF)$_2$ or similar molecules, would break down the paradigm of helium’s inertness.

The article “Metastable He–O bond inside a ferroelectric molecular cavity: (HeO)(LiF)$_2$” will be published in Physical Chemistry Chemical Physics, in a themed issue “Predicting New Molecules by Quantum Chemical Methods” DOI:10.1039/C2CP42321A.