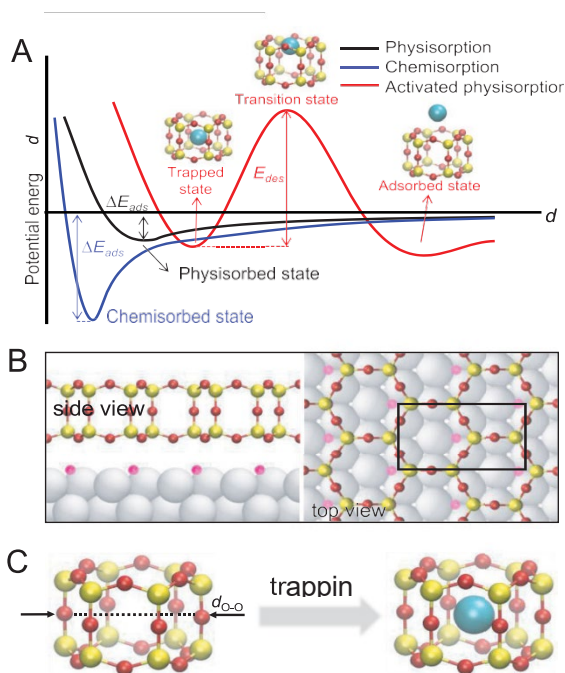


## Xenon Trapping in Silica Nanocages Supported on Metal Powder (Supplemental Document)



**Figure 1.** Potential energy diagram and structure of the 2D silica, as a noble gas atom gets trapped in a nanocage within the structure. A) Schematic diagram of the potential energy for a noble gas against the distance from contact surface ( $d$ ) for physisorption, chemisorption, and activated physisorption, respectively.  $\Delta E_{ads}$  represents the adsorption energy;  $E_{des}$  represents the desorption energy barrier for activated physisorption. B) Side (left) and top (right) views of the 2D silica bilayer film adsorbed on  $p(2 \times 1)\text{-O/Ru}(0001)$  (i.e.,  $(\text{SiO}_2)_8/4\text{O/Ru}(0001)$ ). The black rectangle on the top view indicates the unit cell. C) Illustrations of the nanocages in the framework with and without the noble gas atom trapped inside. Color code: Ru (silver), Si (yellow), O in silica (red), and O chemisorbed on Ru (pink)<sup>8</sup>.

The basic building blocks I have been using in my experiment are called D-POSS (Dodecaphenyl-POSS), which have a hexagonal prism nanocage structure<sup>11</sup>. These are deposited on the porous metal powder of Ru, Co, and Cu. These materials, after various processing steps, are then used to test various conditions for Xe trapping, relevant to applications in nuclear physics and medical isotope production. The work is funded by a BNL LDRD collaborative grant tailored to specifically address these applications.

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