

**4<sup>th</sup> Year Colloquium abstract**

**Submission last date: July 20<sup>th</sup>, 2018**

Presentation title: Using Computer Simulations to Select Simulants for Capture of Chemical Warfare Agents in Nanoporous Materials by Adsorption

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Abstract (150 words maximum, no figures or tables):

Although significant efforts have been made in developing new materials and methods for the adsorption and detoxification of different classes of chemical warfare agents (CWAs), fundamental understanding of the adsorption of such compounds is limited. Among the most promising adsorbent materials in recent years are a class of metal-organic frameworks (MOFs); however, to date little work has been done to systematically probe the relationships between MOF properties and adsorption of CWAs. In this work, we used Monte-Carlo simulations to probe the adsorption of CWAs and simulants in MOFs. Calculated Henry's coefficients were used to first screen the CoRE MOF database of several thousand structures to obtain high performing materials in a series of simulants and CWAs. Our results indicate that not all simulants reliably mimic the behavior of live agents; an important result considering working with live agents is dangerous, costly, and time consuming.