Thermally and Chemically Responsive Nanoporous Materials for Efficient Capture of Fission Product Gases

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ABSTRACT:
This project will create new nanoporous materials that are highly effective for sequestration of fission product gases such as such as He, Xe and Kr in scenarios relevant for both reactor fuels and reprocessing operations. These materials must be radiation tolerant and chemically stable at high temperatures in the presence of reactive species, yet specifically tailored to function efficiently with the target atoms. We will employ molecular dynamics simulations at various interconnected scales to guide identification of appropriate nanostructures which have the optimum shape, size and other material properties for efficient gas capture. The models will be validated using materials with known capture properties, and then expanded to include a wide range of candidate materials to identify those with vastly improved capture properties as well as the required chemical stability and radiation tolerance. Tests will be performed in carbon based and nitride based nanostructures, both with possibility of pore dimensions control using processing conditions. The most promising materials from the modeling perspective shall be synthesized using low-pressure chemical vapor deposition, spark plasma sintering and other complementary methods. Materials will be tested for gas capture efficiency using adsorption-desorption isotherms at different temperatures. Chemical and temperature stability will be examined by exposing the materials to relevant reactive species such as acids and solvents, as well as temperatures up to 1500 °C. Radiation tolerance may be examined in the optimized materials by exposure to ion beams or radioactive isotopes to produce displacement damage effects representative of damage produced by lifetime proximity to nuclear fuels. Preliminary data for response to radiation will also be determined by Molecular Simulations. Materials synthesis, processing, and functional testing will be performed at the University, led by the PI in collaboration with the Faculty Collaborator 1. Simulations will be performed both at the University as well as the National Laboratory, led by Co-PI#1. Key characterization tasks and radiation testing will be led by Co-PI#2 at the National Laboratory. Resources will be divided between the University and the National Laboratory . Two PhD graduate students and two summer undergraduate students will participate in the research. Students that are underrepresented minorities will be recruited for these positions.