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## The theoretical study on the silicide nuclear fuels and cladding materials

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For the nuclear plants, the safety and efficiency of the reactors are the most concerned issues mainly determined by the performance of the applied materials. Hence, the structural design of new nuclear fuels and the development of new generation cladding materials have been the research focus for years. In our works, we have studied the crystalline structures of different members of Uranium silicides by first principle calculations. The impact of defects on the stability and lattice structure of Uranium silicide is investigated and predictions on the performance in the reactor are discussed. As the promising cladding materials, SiC/SiC composite is studied in our group as well. Non-equilibrium Molecular Dynamics simulations are performed to study the mechanism for the mechanical failure of the coating-matrix and coating-fiber interfaces. It is found that the mechanical strength of interface is strongly dependent on the temperature of the system. At 700-1000K, the shear strength is significantly reduced due to the phase transition of the pyrolysis carbon coatings. Furthermore, the implanted He atoms are also determined as a major factor that influences the mechanical behavior. The existence of He atoms in the coating materials may cause a significant increase in shear strength and have a delaying effect on the high temperature failure. By theoretical calculations, we have also found the feasibility of a novel way of space propulsion. According to the results of Monte Carlo simulations, the principle of near-light-speed particle propulsion (NcPP) was raised and the feasibility of applying it for inter-planet travelling was evaluated, which will also be introduced in the presentation.

### Biography

Shiyu Du is a Professor of Material Sciences, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, Zhejiang, China. He got his Doctor's degree (PhD) from Purdue University, USA and did his postdoctoral research on computational material science at Los Alamos National Laboratory, USA. He got Award of Thousand Youth Talents Plan when he started his work in Ningbo, China. Currently, he is working on the national key research and development program of China as the chief scientist. The major research interest of Shiyu Du is on the structural design of nuclear materials by the Materials Genome strategy and the multiscale computational method.

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