



**Theoretical and Physical Chemistry Institute  
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**ONLINE LECTURE**

**“Molecular Dynamics Simulations of Materials at  
Extreme Conditions”**

**Dr. Eva Zarkadoula**

**Materials Science and Technology Division,  
Oak Ridge National Laboratory,  
TN, USA**

**Thursday, November 11, 2021, 15:00**

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# **Molecular Dynamics Simulations of Materials at Extreme Conditions**

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Extreme conditions such as radiation, high temperatures and high stresses are relevant to a plethora of processes and applications from material modification, characterization and synthesis to nuclear environments and the mechanical testing of alloys. Fundamental understanding of the materials' response to extreme conditions is crucial for predicting and controlling the materials' behavior, and for accelerating the design of new systems. In this talk, the importance of understanding the materials' behavior under extreme conditions at the atomistic level will be discussed. Molecular dynamics simulations are a very useful tool for elucidating processes that take place in short length- and timescales, often not accessible by experiment. I will discuss ion-material interactions and the importance of controlling structural defects in material modification with high energy beams and in synthesis with low energy ion implantation, laser beam-material interactions in probing the structure and properties of liquids, and phase transformation of iron-based alloys under stress. Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.