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## Impact of molecular dynamics (MD) simulations in materials research

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To improve awareness of impacts of Molecular Dynamics (MD) simulations on the advancement of materials science and technology, I will give an overview of our molecular dynamics studies of various material problems over the past 10 years. My topics will cover graphene, Giant Magnetoresistive (GMR) multilayers, CdTe/CdS solar cells,  $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$  solid state lighting films, misfit dislocation theory, Al-Cu bond order potential, simulation of chemical reaction involving molecular  $\text{H}_2$  gas, and radiation detecting  $\text{Cd}_{1-x}\text{Zn}_{1-x}\text{Te}$ . In particular, I will show that MD simulations have led to the development of a new million-dollar technology that significantly improved properties of GMR multilayers, and have led to the correction of two parameters in a widely used misfit dislocation theory.

### Biography

X W Zhou completed his PhD from Clemson University, South Carolina, USA. He has been Principal Member of technical staff, Mechanics of Materials Department, Sandia National Laboratories since 2012. He has published more than 100 papers in reputed journals and has been serving as an Editorial Board Member of Journal of Materials Science Research.

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