



COLLEGE OF ENGINEERING AND PHYSICS

Physics Department

PRESENTS A SEMINAR

Atomistic insights into irradiation damage dynamics in metals and alloys

Speaker:



Dr. Qing Peng
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Date: Monday, February 16th, 2026

Time: 11:00 a.m.

Location: Bldg. 6/Room 125

Abstract:

We integrate three atomic-scale simulation studies to elucidate material damage under intense irradiation. (1) Billion-atom molecular dynamics reveals a “punch-out” mechanism where supersonic shockwaves in cascades nucleate $\langle 100 \rangle$ interstitial dislocation loops within picoseconds, highlighting ultrafast defect generation via non-equilibrium energy deposition. (2) Multiscale simulations in NiCoFeCrMn show that chemical short-range order (SRO) evolution under irradiation is governed by a competition between ballistic destruction (depending only on atomic replacements) and element-dependent diffusion-driven recovery. The steady-state SRO can deviate significantly from thermodynamic equilibrium, with important implications for long-term performance. (3) In severely lattice-distorted NbZrTi, first-principles calculations show reduced vacancy/interstitial formation energies, broad vacancy-migration spectra with near-zero barriers, and 3D element-selective interstitial diffusion. These properties enhance point-defect recombination and suppress void swelling under high-temperature irradiation. Together, these studies

provide a multi-scale picture of irradiation damage, from picosecond defect nucleation to long-term microstructural evolution, guiding the design of radiation-resistant materials.

Biography:

Dr. Qing Peng is a Professor (Level 3, senior full professor who serves as a discipline leader) in Wuhan University. He received his PhD from University of Connecticut in 2005, MS from State University of New York at Binghamton in 2000, and BS from Peking University in 1998. His research focuses on computational materials physics using multiscale, first-principles, molecular dynamics, and finite-element modeling and simulations. Dr. Peng has published over 300 peer-reviewed journal papers with over 8600 citations and an H-index of 45. Dr. Peng serves as Editorial board member of a few journals including “Scientific Reports”, “Crystals”, “Nanomaterials”. He is on the Worlds’ Top 2% Scientists list. He is also the Chief Scientific Officer of IC Research Technology (Wuhan) CO. LTD.

. All faculty, researchers and students are invited to attend.



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