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Challenges in Modeling of the Plasma-Material Interface[1] PREDRAG KRSTIC, University of Tennessee, FRED MEYER, Oak Ridge National Laboratory, JEAN PAUL ALLAIN, Purdue University — Plasma-Material Interface mixes materials of the two worlds, creating a new entity, a dynamical surface, which communicates between the two and represent one of the most challenging areas of multidisciplinary science, with many fundamental processes and synergies. How to build an integrated theoretical-experimental approach? Without mutual validation of experiment and theory chances very slim to have believable results? The outreach of the PMI science modeling at the fusion plasma facilities is illustrated by the significant step forward in understanding achieved recently by the quantum-classical modeling of the lithiated carbon surfaces irradiated by deuterium, showing surprisingly large role of oxygen in the deuterium retention and erosion chemistry. The plasma-facing walls of the next-generation fusion reactors will be exposed to high fluxes of neutrons and plasma-particles and will operate at high temperatures for thermodynamic efficiency. To this end we have been studying the evolution dynamics of vacancies and interstitials to the saturated dpa doses of tungsten surfaces bombarded by self-atoms, as well as the plasma-surface interactions of the damaged surfaces (erosion, hydrogen and helium uptake and fuzz formation).

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