Short abstract for **poster presentation** – Carbon 2019

Title: Molecular-Scale Graphene Oxidation and Pitting Dynamics
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Carbon-based heatshield materials are widely used as ablative thermal protection systems (TPS) for hypersonic flight vehicles, e.g. for atmospheric reentry capsules. Such TPS are designed to keep away the extreme aerodynamic heat loads from the underlying vehicle structure by slowly reacting with the ambient oxygen and gasifying as CO and CO2. This oxidation process is not yet well understood, especially its kinetics on the molecular scale and the resulting evolution of the material's nanostructure. We have studied the oxidation dynamics of graphene layers using atomistic simulations. In particular, we developed a kinetic mechanism comprised of the elementary surface processes, coupled with the gas phase by adsorption of oxygen on the graphene layer. This kinetic mechanism has then been employed in kinetic Monte-Carlo simulations to study the oxidation process. Emphasis has been put on the evolution of surface defects, which is typically observed in the form of pitting of the material surface. Our results demonstrate universal features of pitting dynamics as well as the dependence of the pit growth rate on ambient gas conditions.