# Chemistry & Materials with the Amsterdam Modeling Suite Seminar

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**Date and time**
Thursday, March 30 at 10:00 am EDT

**Location**
DLR 131

In this talk, I will give an overview of the Amsterdam Modeling Suite to perform atomistic simulations at various levels of theory. First, I will describe the AMS driver designed to explore potential energy surfaces of molecules and periodic systems, and its integration with our DFT, DFTB and force field engines. To illustrate the capability of our DFT engines, I will introduce a few studies performed with ADF and its periodic extension BAND. Second, I will focus on force fields (ReaxFF and MLPotential) to describe reactive systems and polymer chemistry. Finally, I will present PARAMS to create new force field parameters in order to describe novel molecular interactions. Along with this presentation, I will illustrate the various applications with short demos or videos performed with the AMS graphical user interface.

Dr. Nicolas Onofrio received his Ph.D. from the department of Chemistry at the University of Grenoble Alpes in France followed by a Postdoc at Purdue University. Dr. Onofrio was an Assistant Professor in the department of Applied Physics at the Hong Kong Polytechnic University before joining SCM in 2023.

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