

# NOMATEN JUNIOR SEMINAR

Tuesday, March 8, 2022 13:00 (1.00PM CET)

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## Many-body van der Waals interactions beyond the dipole approximation

Dario Massa PhD, NOMATEN CoE, Materials Informatics Structure and Function Research Group; NCBJ

### **Abstract:**

Long-ranged van der Waals (vdW) interactions are most often treated via Lennard-Jones approaches based on the combination of two-body and dipolar approximations. While beyond-dipole interactions and many-body contributions were separately addressed, little is known about their combined effect, especially in large molecules and relevant nanoscale systems. In this work, a full many-body description of vdW interactions beyond the dipole approximation is provided, efficiently applicable to large-scale systems. Dipole–quadrupole interactions consistently exhibit large magnitude up to nm-scale separations, while many-body effects lead to system-dependent screening effects, which can reduce vdW interactions by a large fraction. Combined many-body and multipolar terms emerge as an essential ingredient for the reliable description of vdW interactions in molecular and nanoscale systems."

### **Bio:**

Dario Massa has attained his Bachelor degree in Physics at the University of Roma La Sapienza and his M.Sc. degree in Physics at the University of Padua, Italy. He has carried on a 9-months research project at the University of Padua on vdW interactions modeling. Recently has been accepted as a PhD assistant at NCBJ in the group of Dr./Prof. Papanikolaou's, where he has started working on his project in alloy informatics for hydrogen storage.