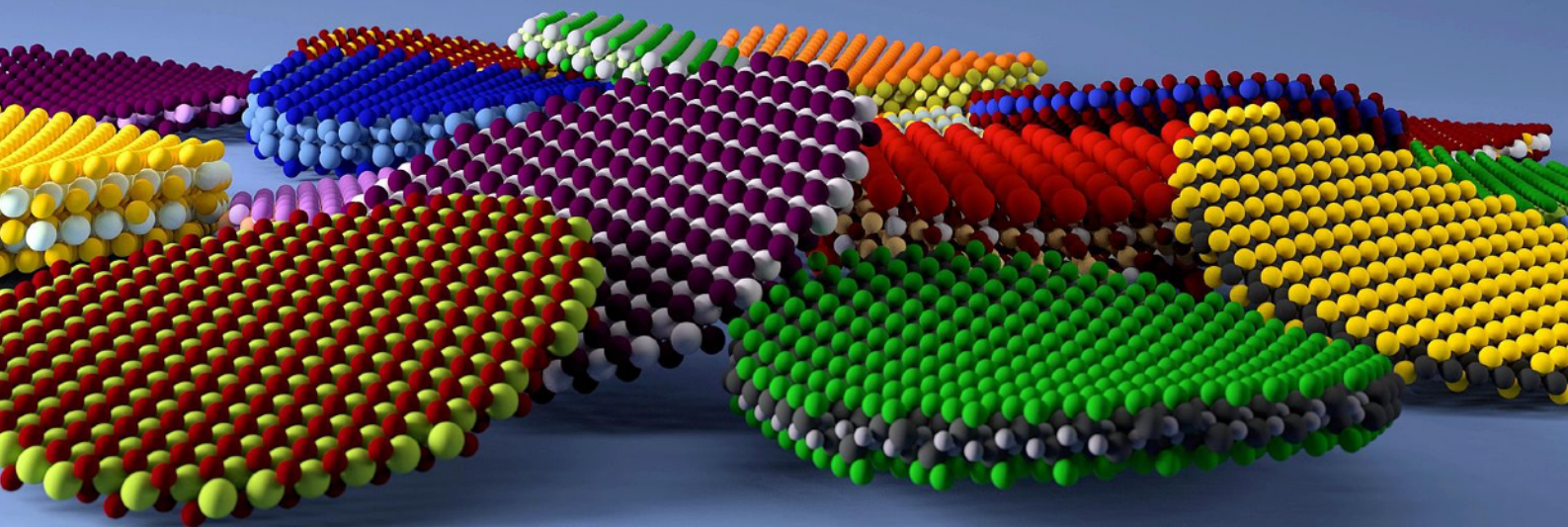




Is there really room at the bottom?

Novel 2D materials from computational exfoliation



Dr. Antimo Marrazzo
Physics Department,
University of Trieste

Monday June 28th 2021
16:30-17:30

Room A, building F
Via Valerio 2, Trieste



Also on Zoom at
<https://tinyurl.com/2Dseminar>
Meeting ID: 986 3143 0170
Passcode: 2Dmat

Since the discovery of graphene in 2004, two-dimensional materials have seen a steady growth in experimental and theoretical efforts, searching for novel physics and functionalities.

In this talk, I will present a systematic exploration of all known inorganic materials through first-principles simulations and materials informatics, to identify candidates that could be exfoliated into two-dimensional monolayers. Remarkably, we found about 2000 inorganic compounds that could be exfoliated into novel two-dimensional materials, and recover in the process all known ones, such as graphene, transition-metal dichalcogenides, boron nitride and more.

I will start with a pedagogical introduction to van-der-Waals materials and density-functional theory, before discussing the high-throughput approach to computational materials discovery and the subtleties of calculating properties for two-dimensional structures. Then, I will present our portfolio of exfoliable materials and conclude by providing a broad perspective on the promising properties that we are uncovering, with examples targeting electronics and spintronics applications.