



University of Crete  
Department of Physics

## *Physics Colloquium*

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Thursday, 26 November 2020 | 17:00 – 18:00, Online with BBB

# **Designing 2D (hetero)structures through computational modeling**

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### **ABSTRACT**

*The rich variety of two-dimensional (2D) structures, both in type and phase, sets a wonderful framework for a tailored design of novel nanostructures with selected properties. With this in mind and the aid of computational modeling, we suggest and investigate various 2D (hetero)structures in view of tuning their optoelectronic and transport properties. Using on top of the simulations also Machine Learning algorithms further allows the prediction on the adsorption of atomic species on the 2D materials. The detailed insight gained from our modeling approaches allows us to propose novel applications in nanoelectronics and (bio)molecular sensing.*