



Institute for Materials Science, Chair of Materials Science and nanotechnology

3<sup>rd</sup> TAC Meeting

# **Computational studies of electronic and thermal properties of low dimensional materials**

**Rodriguez Mendez Alvaro Gaspar** 

22.03.2023

#### **Thesis Content**

I. Introduction

II. Methodology

Density Functional Theroy

DFTB

Atomistic Green's Functions

III. Tuning the electronic and magnetic properties through chemical functionalization

IV. Tuning transport properties through strain and grain boundaries

V. Tuning transport properties through hybrid nanomaterials: CNT peapods







## Functionalizing phosphorene towards bipolar magnetic semiconductors





Rodriguez Mendez Alvaro Gaspar Chair of Materials Science and Nanotechnology Computational studies of electronic and thermal properties of low dimensional materials





### **Electronic and Thermal Signatures of Phosphorene Grain Boundaries under Uniaxial Strain**





Rodriguez Mendez Alvaro Gaspar Chair of Materials Science and Nanotechnology Computational studies of electronic and thermal properties of low dimensional materials





### An Atomistic Study of the Thermoelectric Signatures of CNT Peapods





Rodriguez Mendez Alvaro Gaspar Chair of Materials Science and Nanotechnology Computational studies of electronic and thermal properties of low dimensional materials



