Α ΡΙΣΤΟΤΕΛΕΙΟ
Π ΑΝΕΠΙΣΤΗΜΙΟ
Θ ΕΣΣΑΛΟΝΙΚΗΣ

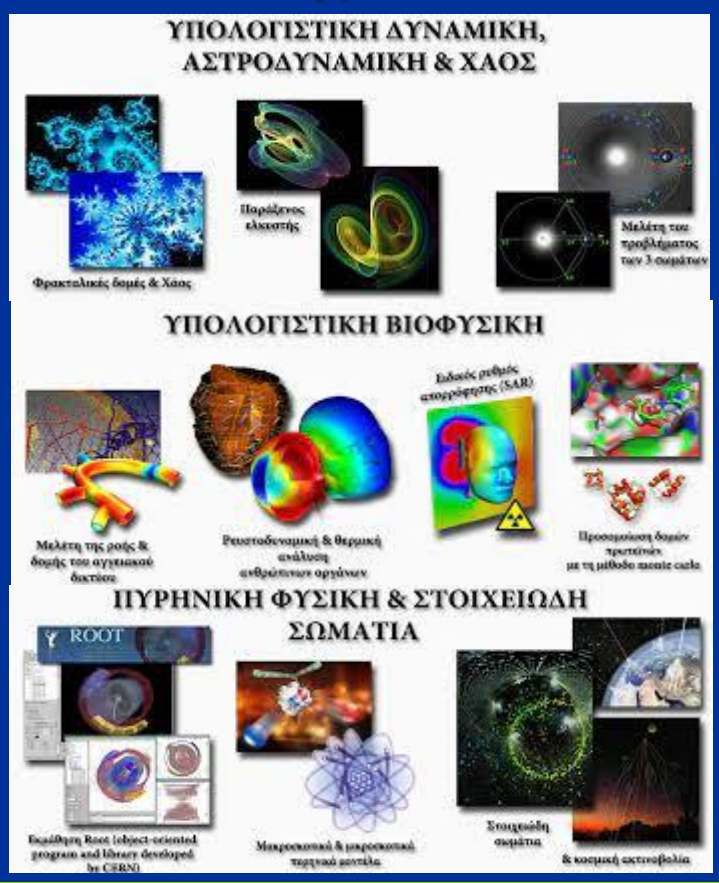
ΣΕΜΙΝΑΡΙΟ
ΠΜΣ ΥΠΟΛΟΓΙΣΤΙΚΗΣ ΦΥΣΙΚΗΣ
ΤΜΗΜΑ ΦΥΣΙΚΗΣ

Τετάρτη 13 Απριλίου 2022

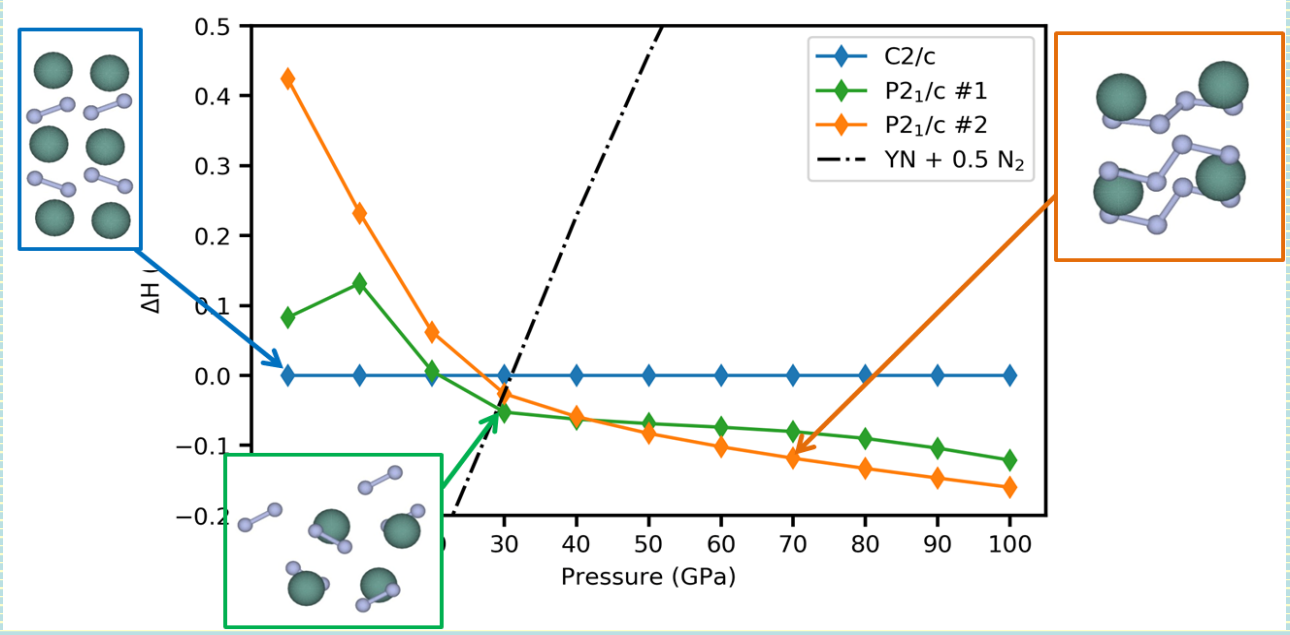
ώρα 13:00

Αίθουσα Α31

Σεμινάρια ΠΜΣ Υπολογιστικής Φυσικής 2021-2022



Crystal Structure Prediction and Beyond



Davide Ceresoli

CNR-SCITEC, Milan, Italy

The focus of my talk will be the computational prediction of new materials that are formed in the planets interior, or that can be synthesized at high pressure in the lab. I will present three different strategies to predict new compounds under pressure: (1) explore known prototypes; (2) global optimization via evolutionary algorithms; (3) data mining and high-throughput calculations. Then I will shortly discuss the long route to predict "how to synthesize new materials". All calculations are performed with Density Functional Theory.

Το προφίλ του ομιλητή

Davide Ceresoli is a senior researcher at CNR-SCITEC in Milan since 2020. He studied Materials Science at the University of Milan-Bicocca and in 2002 he got his PhD in Physics at SISSA, Trieste, Italy, working on Berry phases in molecules and solids. Since then he has been postdoc at Rutgers University, SISSA, MIT and Oxford University. In 2011 he became researcher at CNR-ISTM in Milan. His main research interests are theory of orbital magnetization, materials modeling in collaboration with industry, and recently, high pressure simulation of materials and phase transitions. He is one of the developer of Quantum Espresso (QE), QE-GIPAW and related codes.