



Università «G d'Annunzio» Chieti-Pescara

Dipartimento di Farmacia

Scuola Superiore «G. d'Annunzio»

Experiment-Theory: a round trip

«A focus on chemical studies at the interface between experiment and theory»

14 settembre 2023 - ore 9:00

Aula multimediale del campus di Chieti

Speakers

Richard H. Fish

Lawrence Berkeley National Laboratory, UC Berkeley (USA)

Alessandro Marrone

Dipartimento di Farmacia, (UdA)

Nicola D'Alessandro

Dipartimento INGEO, SBF (UdA)

Corrado Di Nicola

Scuola di Scienze e Tecnologie, (Unicam)

Cecilia Coletti

Dipartimento di Farmacia, SBF (UdA)

Pietro Di Profio

Dipartimento di Farmacia, SBF (UdA)

Loriano Storchi

Dipartimento di Farmacia, SBF (UdA)





Program

9:00

Alessandro Marrone
Dipartimento di Farmacia, (UdA)

Opening

9:15

Richard H. Fish
Lawrence Berkeley National Laboratory, UC Berkeley (USA)

Bioorganometallic Chemistry: Biocatalysis and Organometallic Pharmaceutical Studies, GPCR Peptide Reactions with $[\text{Cp}^*\text{Rh}(\text{H}_2\text{O})_3](\text{OTf})_2$, Host-Guest Recognition, Synthesis and X-Ray Structures of $[\text{Cp}^*\text{Rh}\text{-DNA}]$ Complexes, and Including DFT and MD Computational Studies.

10:00

Cecilia Coletti
Dipartimento di Farmacia, SBF (UdA)

Structure and dynamics of ions in gas phase: interplay between experiments and theory in IR action spectroscopy.

10:25

Loriano Storchi
Dipartimento di Farmacia, SBF (UdA)

Machine and Deep Learning techniques in chemistry: from DeepGRID to a simple formula generator.

11:15

Corrado Di Nicola
Scuola di Scienze e Tecnologie, (Unicam)

Pyrazolate-based MOFs for CO_2 capture and utilization.

11:35

Nicola D'Alessandro
Dipartimento INGEO, SBF (UdA)

Rhenium catalyzed deoxydehydration reaction to obtain alkenes

11:50

Pietro Di Profio
Dipartimento di Farmacia, SBF (UdA)

Three cases of mismatch between empirical models and experiments in the field of clathrate hydrates.