032CM - 2025

PROGRAMMING FOR COMPUTATIONAL CHEMISTRY

Presentations

Gianluca Levi

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Office: Building C11, 3rd floor, Room 329

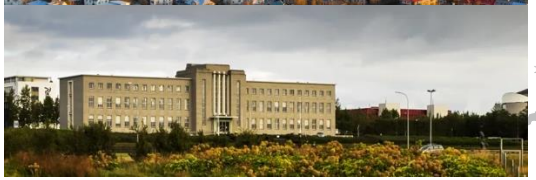
Fall 2025

University of Naples Federico II
MSc in Chemistry (2014)

Technical University of Denmark
PhD in Theoretical Physical Chemistry (2018)

University of Naples Federico II
MSc in Chemistry (2014)

University of Iceland
Postdoc (2018 - 2024)
Res. Assoc. Professor (2025 -)



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Res. Assoc. Professor (2025 -)
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PhD in Theoretical Physical Chemistry (2018)
University of Naples Federico II
MSc in Chemistry (2014)
University of Trieste
Assoc. Professor (2025 -)

My teaching

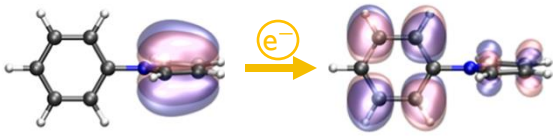
Courses for graduate and undergraduate students in chemistry, biochemistry and chemical engineering

2022 -	**Molecular Spectroscopy and Reaction Dynamics** **Physical Chemistry A** **Computational Chemistry** Department of Chemistry, University of Iceland
2023	**Molecular Dynamics and X-ray Scattering Simulations** Department of Physics, Technical University of Denmark
2015 - 2016	**Physical Chemistry 3** **Applied Computational Chemistry** Department of Chemistry, Technical University of Denmark

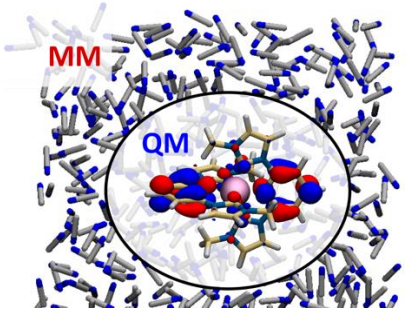
My research activities

Development of methodologies for modelling **excited electronic states** of molecules and materials

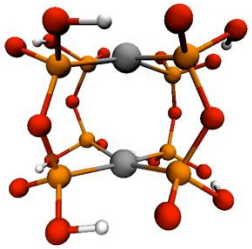
$$\left[-\frac{1}{2}\nabla^2 + \hat{v} + \hat{v}_{\text{eff}}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$



Development of multiscale and **molecular dynamics** methods



$$\ddot{\mathbf{R}}_\alpha = -\frac{\nabla_\alpha E_i}{M_\alpha}$$



$$\hat{H}_{\text{e}}^{\text{eff}} = \hat{H}_{\text{QM}} + \hat{H}_{\text{QM/MM}} + \hat{H}_{\text{MM}}$$

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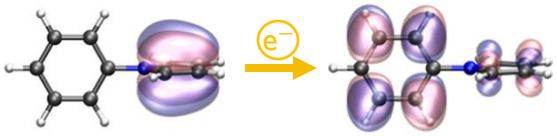

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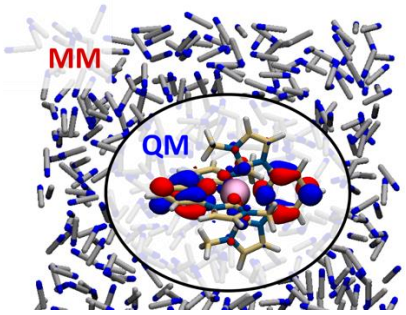

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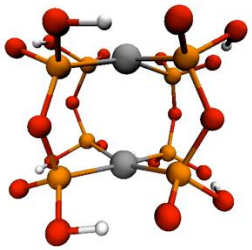

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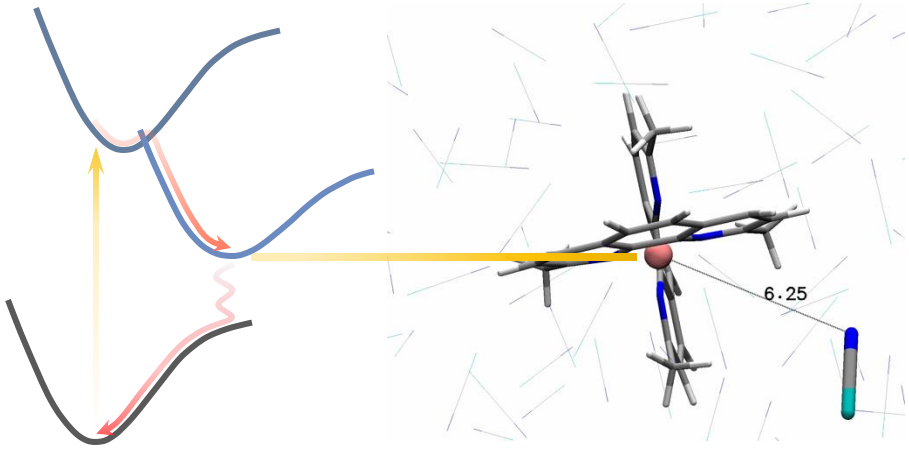
Atomic-scale simulations of systems for **solar energy conversion and catalysis**



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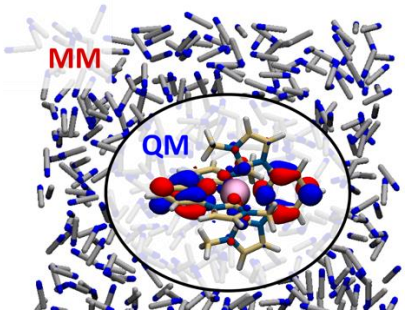

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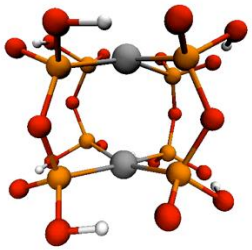

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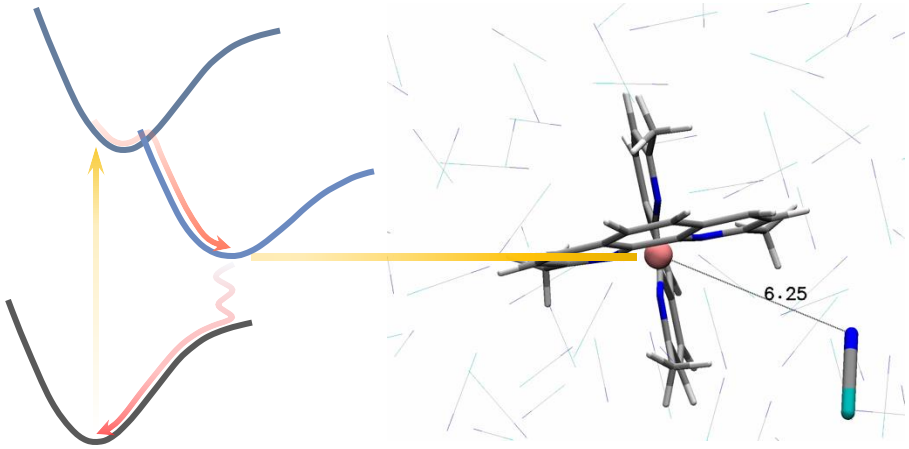

Time-resolved spectroscopy and X-ray scattering **experiments** at large-scale facilities