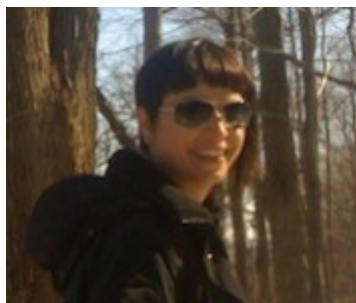


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# POMÈS LAB

Computational Biophysics: Biomacromolecular Structure, Function, and Dynamics



## Elisa Fadda

Elisa is a senior research fellow in Robert J. Woods lab in the Department of Chemistry at the National University of Ireland in Galway, where she manages the computational lab. One of the main focuses of her research is gaining insight into the structure, dynamics, and energetics of carbohydrate-protein interactions through computational methods.

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### **Brief Biography**

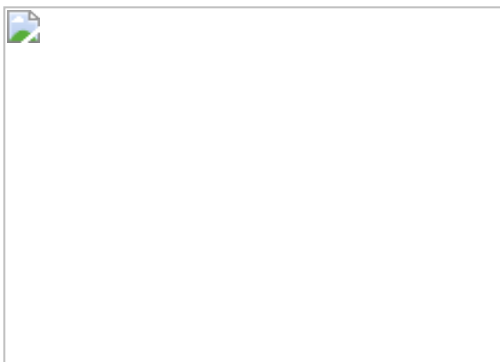
- B.Sc. and M.Sc.(Laurea) in Physical Chemistry; Università degli Studi di Cagliari, Cagliari (Italy)
- Ph.D. in Theoretical and Computational Chemistry; Université de Montréal, Montréal (Canada)
- Post-Doctoral Fellow in Computational Chemistry, Molecular Structure and Function, The Hospital for Sick Children, Toronto (Canada)

### **Research Areas:**

- QM/MM study of the pumping mechanism of cytochrome c oxidase
- Classical and QM/MM free-energy calculations on proton transport in natural and biomimetic protein channels
- Design and thermodynamic stability (QM) of new Cu(II)-transporters (project in collaboration with Prof. Nohad Gresh, Université Paris V René Descartes, Paris, France)
- QM and QM/MM Study of the Reaction Mechanism of alpha-Golgi Mannosidase II (GMII) (in collaboration with Dr. S. Kawatkar and Dr. R.J. Woods)

## Publications:

1. E. Fadda, C.-H. Yu, R. Pomès. "Electrostatic Control of Proton Pumping in Cytochrome c Oxidase", Biophys. Biochim. Acta, Bioenergetics, 1777, 277 (2008)
2. E. Fadda, N. Chakrabarti, and R. Pomès "Reply to the Comment on "Acidity of a Cu-Bound Histidine in the Binuclear Center of Cytochrome c Oxidase" J. Phys. Chem. B, 110, 17288 (2006)
3. E. Fadda, N. Chakrabarti, and R. Pomès "Acidity of a Cu-Bound Histidine in the Binuclear Center of Cytochrome c Oxidase" J. Phys. Chem. B, 109, 22629 (2005)
4. E. Fadda, M.E. Casida and D.R. Salahub: "14,15N NMR Shielding Constants from Density-Functional Theory", J. Phys. Chem. A, 107, 9924 (2003)
5. E.Fadda, M.E. Casida, and D.R. Salahub: "NMR Shieldings from Sum-Over-States Density-Functional Perturbation-Theory: Further Testing of the "Loc.3" Approximation", J. Chem. Phys., 118, 6758 (2003)
6. E.Fadda, M.E. Casida, and D.R. Salahub: "Time-Dependent Density-Functional Theory as a Foundation for a Firmer Understanding of Sum-Over-States Density-Functional Perturbation-Theory: "Loc.3" Approximation", Int. J. Quantum. Chem., 91, 68 (2003)



## Group - Alumni

- [Aditi Ramesh](#) - MSc
- [Adrian Levine](#) - Researcher
- [Ana Nikolic](#) - Researcher
- [Ching-Hsing Yu](#) - Researcher
- [Chris Madill](#) - PhD
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- [Sarah Rauscher](#) - PhD
- [Stéphanie Baud](#) - Postdoctoral Fellow
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## Funding

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