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POMËS LAB

Computational Biophysics: Biomacromolecular Structure, Function, and Dynamics



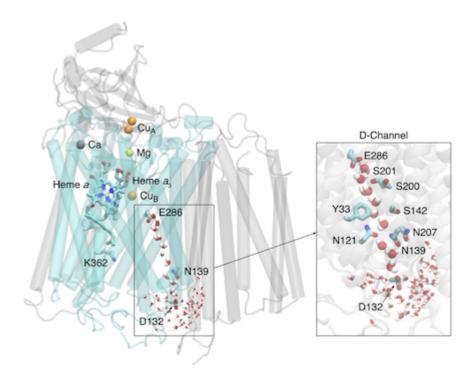
Christopher Ing

I aim to understand the biophysical mechanisms of wild-type and mutant <u>cytochrome c oxidase</u> using all-atom molecular dynamics. I am particularly interested in ion movement and solvation in these proteins.

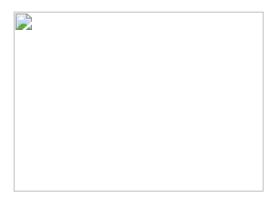
Research Interests

Under the guidance of <u>Dr. Pierre Nicholas Roy</u>, I calculated properties of small quantum clusters systems at ultra low temperatures. To achieve this I utilized a path integral molecular dynamics sampling method which I assisted in implementing in the <u>Molecular Modelling Toolkit</u>. The simulation of path integral helium about a fixed CO2 impurity is <u>shown here</u> for a 64 time-slice helium atom.

In my current research, I aim to advance research in the Pomès Lab on the molecular structure and function of cytochrome c oxidase. Cytochrome c oxidase of R. sphaeroides is depicted in the following figure from J. Phys.: Condens. Matter **23** (2011) 234102. Subunit I, which contains the D channel (inset) and the binuclear centre, highlighted in blue. These are the primary regions of importance to electron and proton transport.



I am also actively involved in studying the molecular structure and function of other membrane proteins like the voltage-gated sodium channel. I am currently working on Python software to assist in the analysis of timeseries data from multiple simulation repeats.



Group - Alumni

- Régis Pomès Principal investigator
- Ananya Srivastava MSc
- Anna Liang MSc
- Christopher Ing PhD Candidate
- Jingjing Huang PhD Candidate
- Quang Huynh MSc
- Richard Banh Researcher
- Zhi Zeng MSc

Contact

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- Canadian Institutes of Health Research
- Natural Science and Engineering Research Council
- National Institutes of Health
- Canadian Foundation for Innovation

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