

Applications are invited for a postdoctoral position in theoretical/computational chemistry (quantum dynamics of molecules and clusters) in the group of Prof. Tucker Carrington. The position is available immediately, but the starting date is flexible. The initial appointment will be for one year, renewable for one or possibly two years upon mutual consent.

Current research areas are:

- (a) The development and application of contracted basis Lanczos methods to compute ro-vibrational spectra of polyatomic molecules. Relevant references:

J. Chem. Phys. **125**, 094311-1--094311-12 (2006)

Physical Review Letters **98**, 119301.(2007)

J. Chem. Phys. **122**, 244107--1-244107-11 (2005).

J. Chem. Phys. **123** 034301-1—034301-15 (2005).

J. Chem. Phys. **121** 2937-2954 (2004).

J. Chem. Phys. **119**, 101-117 (2003).

- (b) Using simultaneous diagonalisation to make efficient phase-space localized basis sets for studying quantum dynamics. See for example,

J. Chem. Phys. **124**, 054102-1-- 054102-11 (2006).

J. Chem. Phys. . **122** 134101-1—134101-14 (2005).

- (c) The use of neural networks both to represent potentials and to solve the Schrödinger equation. Relevant references are:

J. Chem. Phys. **127**, 014103-1 -- 014103-10 (2007)

J. Chem. Phys. **125**, 194105-1--194105-5 (2006).

J. Chem. Phys. **125**, 084109-1--084109-14 (2006).

J. Phys. Chem. **110** (John Light Festschrift), 5295-5304 (2006).

The work involves method and code development, and large-scale calculations. Highly motivated candidates with a desire to excel, programming experience, good mathematical skills, and a good background in quantum mechanics, theoretical chemistry, classical and quantum dynamics, and related fields are encouraged to apply.

Please feel free to contact me for further details.

To apply, please send, preferably by e-mail, a CV, list of publications, and arrange for three letters of recommendation to be sent directly to the address below (e-mail is preferred).

Tucker Carrington
Chemistry Department
Queen's University
Kingston, Ontario
K7L 3N6
Canada

|-----|
tel: (613) 533-2552
e-mail: Tucker.Carrington@chem.queensu.ca
fax: 613-533-6669
<http://www.chem.queensu.ca/people/faculty/Carrington/index.asp>