

# Pacificchem 2010

Announcing the **Fourth OF-DFT Symposium at Pacificchem 2010**  
in the Topic Area of *Physical, Theoretical & Computational*, on **Dec. 19-20**.

## Orbital-Free Density Functional Theory and Its Applications to Large-Scale Materials Simulations (#05.258)

Organized by: Yan Alexander Wang (UBC, Canada) <[yawang@chem.ubc.ca](mailto:yawang@chem.ubc.ca)>  
Tomasz A. Wesolowski (Geneva, Switzerland)  
Julian D. Gale (Curtin, Australia)  
Carlos J. Garcia-Cervera (UC Santa Barbara, USA)

In the last decade, there has been a revival of orbital-free density functional theory (OF-DFT), pioneered by Thomas and Fermi as the first generation of DFT in the late 1930's. OF-DFT is quite appealing in that its computational cost is essentially linear,  $O(N \ln N)$ , for a given numerical grid size  $N$ . This feature makes it a powerful tool for large-scale materials simulations with thousands of atoms involved. Unfortunately, the early days of OF-DFT suffered from poor design of the kinetic-energy density functional (KEDF). Not until the late 1990's, high-quality orbital-free KEDFs began to emerge. Despite the fact that many materials simulations have been performed with OF-DFT methods, certain mathematical issues in the design of the KEDF and several major obstacles remain unresolved before OF-DFT becomes a main-stream *ab initio* simulation method. For the fourth time, mathematicians, functional designers, methodology developers, and method practitioners will come together to showcase recent developments in OF-DFT and to position OF-DFT as a major tool in simulating complex systems of thousands of atoms within a diverse chemical bonding environment.

### Speakers and Session Chairs:

Andrés Aguado (Spain)	David J. Gonzalez (Spain)	Johannes Neugebauer (Netherlands)
Jose E. Alvarelos (Spain)	Luis E. Gonzalez (Spain)	Daniel Neuhauser (USA)
Paul W. Ayers (Canada)	Oleg V. Gritsenko (Netherlands)	Sture Nordholm (Sweden)
Kieron Burke (USA)	Ian P. Hamilton (Canada)	Stefano Pittalis (USA)
Eric Cancès (France)	Miroslav Hodak (USA)	Octavio Roncero (Spain)
Emily A. Carter (USA)	Chen Huang (USA)	Paul J. Scott (Canada)
Guanhua Chen (Hong Kong)	Christoph Jacob (Germany)	Lucas Visscher (Netherlands)
Peter Elliott (USA)	Valentin V. Karasiev (USA)	Yan Alexander Wang (Canada)
Julian D. Gale (Australia)	Uzi Landman (USA)	Adam Wasserman (USA)
Weiguo Gao (China)	Jose-Manuel López (Spain)	Tomasz A. Wesolowski (Switzerland)
Carlos J. Garcia-Cervera (USA)	Gang Lu (USA)	Weitao Yang (USA)
Vikram Gavini (USA)	Agnes Nagy (Hungary)	Constantine Yannouleas (USA)

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