SCIENCES &
BIOENGINEERING SCIENCES

The Research Group
General Chemistry

has the honor to invite you to the public defence of the PhD thesis of

Bin Wang

to obtain the degree of Doctor of Sciences

Title of the PhD thesis:

Towards Analytical Conceptual Density Functional Theory: Fundamentals, Implementation and Applications

Supervisors:
Prof. dr. Frank De Proft (VUB)
Em. prof. dr. Paul Geerlings (VUB)
Co-supervisor:
Prof. dr. Shubin Liu (University of North Carolina, USA)

The defence will take place on

Wednesday, September 10, 2025 at 5 p.m.

VUB Etterbeek campus, Pleinlaan 2, Elsene,
auditorium I.0.01

The defence can be followed through a live stream: contact Bin Wang for more information.

Members of the jury

Prof. dr. Frederik Tielens (VUB, chair)
Prof. dr. Mercedes Alonso Giner (VUB)
Prof. dr. Dominique Maes (VUB)
Prof. dr. Mark Sioen (VUB)
Dr. Julia Contreras-Garcia (Sorbonne Université & CNRS, FR)
Prof. dr. Christophe Morell (Université de Lyon, FR)
Prof. dr. Andrew M. Wibowo-Teale (University of Nottingham, UK)

Curriculum vitae

Bin Wang obtained his four years BSc program degree from the Hunan Normal University in 2021. He then started his doctoral research at Gereral Chemistry research group (ALGC) at the VUB funded by the Chinese scholarship council.

He has published six first-authored, peer-reviewed papers and has given one oral presentation and five poster presentations at international conferences during his PhD program. In addition to other teaching activities, he has also supervised one bachelor's thesis and one master's thesis.

Abstract of the PhD research

Conceptual density functional theory (CDFT), derived from density functional theory (DFT), provides a robust framework for understanding chemical reactivity, linking chemical concepts with fundamental physics. Through the introduction of so-called response functions, CDFT rigorously defines several well-known but previously vaguely defined concepts, such as electronic chemical potential (electronegativity), hardness, softness, and others.

This PhD research focuses on the analytical development of CDFT, providing a clear and detailed derivation and implementation of each of these response functions up to second order. Numerical differences between the widely used approximations of these response functions (using the frontier molecular orbitals or the finite difference approximation) and the analytical ones obtained through the Coupled-Perturbed Kohn-Sham scheme have been carefully examined. Besides improving the prediction of the chemical selectivity using traditional CDFT and realizing analyses that are previously impractical, e.g. decomposing reactivity into population normal modes, the analytical evaluation also opens the room for investigating the fundamental failures of DFT e.g. the delocalization error of modern density functional approximations (DFAs). Next, an extension to chemical bond resolution through the newly introduced conceptual density matrix functional theory (CDMFT) is presented. CDMFT offers a new perspective for exploring bond reactivity, including the description of bond-bond polarizability. An important application of CDMFT is demonstrated through the simulation of primary bond cleavage in electron impact mass spectrometry using response properties. Furthermore, a method is proposed for automatically evaluating arbitrary order of response functions without explicitly addressing the coupled perturbed self-consistent field equations. In a final part, through the combination of CDFT and concepts from the information-theoretic approach in DFT, a new reactivity partitioning method of the reaction coordinate of an elementary reaction step is proposed to divide the full reaction path into segments that are individually controlled by physically meaningful factors such as electrophilicity/nucleophilicity and steric effects.