

Séminaire de Chimie Théorique

Salle conference 3eme Est, Bat. A12

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Large Scale Electronic Structure Calculations: The CONQUEST code and Nanostructures

Linear scaling or $O(N)$ electronic structure codes have been under development for around fifteen years^[1]. The CONQUEST code^[2] is one of the leading $O(N)$ codes, and has demonstrated not only excellent scaling to over two million atoms and many thousands of cores^[3] but also practical applications to nanostructures on semiconductor surfaces^[4]. I will describe the CONQUEST code, along with recent improvements including constrained DFT^[5] and TDDFT, and discuss its implementation. I will also present results on simulations of nanostructures on semiconductor surfaces, both with CONQUEST and other linear scaling approaches.

[1] D. R. Bowler and T. Miyazaki, Rep. Prog. Phys. 75 036503 (2012)

[2] D. R. Bowler, R. Choudhury, M. J. Gillan and T. Miyazaki, phys. stat. sol. b 243 989-1000 (2006)

[3] D. R. Bowler and T. Miyazaki, J. Phys.: Condens. Matter 22 074207 (2010)

[4] T. Miyazaki, D. R. Bowler, M. J. Gillan and T. Ohno, J. Phys. Soc. Jpn. 77 123706 (2008)

[5] A. M. P. Sena, T. Miyazaki and D. R. Bowler, J. Chem. Theory Comput. 7 884-889 (2011)

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