SYLLABUS

2022 Summer School on Electronic Structure Calculations Using GFN2-xTB

Course Description

This course will first give a general introduction on computational chemistry/materials science, including various length and time scales. We will then focus on one specific semiempirical method, extended tight-binding (GFN2-xTB)[1], of electronic structure calculations. The reason for choosing this method is because (1) it is efficient (capable of running on even laptop), and (2) it has reasonable predicting power for molecular geometry. And, most importantly, it is free. We will go through several examples that are common practice in quantum chemistry package (such as GAUSSIAN[2]).

Teaching Method

Lecture using ppt slides + hands-on session. It will be roughly 4~5 hours a week every Friday afternoon.

Course Requirements

- Participants should prepare their own laptops and install the prerequisites, including Linux operating system (Ubuntu 16.04 recommended), visualization software (Avogadro and Molden) and the xTB code.
- There will be homework every week and the due day is one day before the next course. Participants are required to hand in the homework; otherwise they are not eligible to follow the rest of the course.

Readings

Molecular Quantum Mechanics 5th Ed., Peter Atkins
Essentials of Computational Chemistry: Theories and Models, Christopher J. Cramer
Introduction to Computational Chemistry, Frank Jensen

Calendar

Week	Topics	Key dates
1 08/07	Introduction to computational chemistry & geometry optimization (HW1)	

2 15/07	Molecular orbitals & molecular properties (HW2)	HW1 due
3 22/07	Electrostatic potential & intermolecular interactions (HW3)	HW2 due
4 29/07	NO COURSE	
5 05/08	NO COURSE	
6 29/07	Vibrational frequency & IR/Raman spectrum (HW4)	HW3 due
7 12/08	Vibrational frequency & thermodynamic properties (HW5)	HW4 due
8 19/08	Molecular dynamics & conformational search (HW6)	HW5 due
9 26/08	Solvation energy with implicit solvent model	HW6 due

Reference

1 C. Bannwarth, S. Ehlert and S. Grimme, *J. Chem. Theory Comput.*, 2019, **15**, 1652–1671.

2 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, J. E. P. Jr., F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R.

L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, 2016, Gaussian, Inc., Wallingford CT.