密度泛函理論 （學分數:2, 授課老師:蔡政達）

上課時間(教室):星期一34(新物304)

課程網頁:進入 http://web.phys.ntu.edu.tw/jdchai/courses.html 後,
點選右側 [1] Density Functional Theory 或直接進入 https://cool.ntu.edu.tw/courses/41922

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作業共 2 份, 以英文出題。作業抄襲者及給人抄襲者, 該題以不計分論。
作業成績:30%
口頭報告:20%
書面報告:50% (題目需於10/21前選定)

教科書: 以上課筆記為主。
參考書 (非必要):
1. R. G. Parr and W. Yang, “Density Functional Theory of Atoms and Molecules” (Oxford University Press, New York, 1989).
2. J. Kohanoff, “Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods” (Cambridge University Press, New York, 2006).
3. F. Jensen, “Introduction to Computational Chemistry” (Wiley, New York, 2007).
4. M. E. Casida, “Recent Advances in Density Functional Methods”, Part I (World Scientific, Singapore, 1995).
5. E. K. U. Gross, J. F. Dobson, and M. Petersilka, “Density Functional Theory II” (Springer, Heidelberg, 1996).
6. E. Engel and R. M. Dreizler, “Density Functional Theory: An Advanced Course” (Springer, Heidelberg, 2011).

課程大綱:
09/02 Schrödinger Equation
09/09 Hartree-Fock Equation (and Beyond)
09/16 Thomas-Fermi Model (and Beyond)
09/23 Hohenberg-Kohn Theorem
09/30 Kohn-Sham Equation
10/07 Exchange-Correlation Energy Functional
10/14 Local Density Approximation (and Beyond)
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10/21 Hybrid Density Functionals
10/28 Double-Hybrid Density Functionals
11/04 Time-Dependent DFT
11/11 Excited States
11/18 Advanced Topics in DFT
---------- 作業2
11/25 口頭報告1 (10:20~12:00)
12/02 口頭報告2 (10:20~12:00)
12/09 口頭報告3 (10:20~12:00)
12/19 書面報告繳交截止日