INTERMOLECULAR INTERACTIONS
Theory and Electronic Structure Methods

Quantum Chemistry & Molecular Modeling Group

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Description: This short course provides a concise introduction to the quantum theory of intermolecular interactions and its calculation by the elctronic structure methods.

Contents:

Lecture 1	(ARM)	:	Introduction to intermolecular interactions.
Lecture 2	(ARM)	:	Molecular quantum mechanics.
Lecture 3	(ARM)	:	Quantum nature of intermolecular interactions.
Lecture 4	(SFG)	:	Ab-initio calculation of intermolecular interactions.
LAB	(SFG)	:	Computational laboratory sesion.

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Evaluation: Attendance and individual work.

Bibliography:

[1] P. Atkins & J. de Paula, Physical Chemistry, 9th Ed, W. H. Freeman and Company, New York, 2010.
[2] P. Atkins & R. Friedman, Molecular Quantum Mechanics, 4th Ed, Oxford University Press, Oxford, 2005.
[3] A.J. Stone, The Theory of Intermolecular Forces, 2nd Ed, Oxford University Press, Oxford, 2013.
[4] I.G. Kaplan, Intermolecular Interactions, John Wiley & Sons, Chichester UK, 2006.