UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

Syllabus 2020/21

Teacher (name and affiliation)	Piercarlo Fantucci (UNIMIB-DISAT)
Title	Separability in quantum chemistry and effective potential theories
Language	English
CFU	2.5
Hours	20
Program	The general problem of separability in quantum chemistry. Groups of electrons and their interaction. The orthogonality problem. Sigma-Pi separability. Core-Valence separability. The need of effective core-valence potentials (ECP). Core-valence interaction in heavy atoms and relativistic effects. Objectives of the program: Understanding the theoretical background of using the ECP approach in computational quantum chemistry. What it can be computed (and what not) on the basis of ECP approaches. ECP for molecular systems and solid-state-like systems.

Evaluation: YES/NO	Yes
Calendar	1st semester