



UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Separability in Quantum Chemistry and Effective Potential Theories (Curricular - Chemistry)

2021-94R-SCGA14

Titolo

Separability in quantum chemistry and effective potential theories

Docente(i)

Piercarlo Fantucci

Lingua

English

Breve descrizione

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

CFU / Ore

2,5 CFU - 20 Hours (Lecture)

Periodo di erogazione

Il semester
