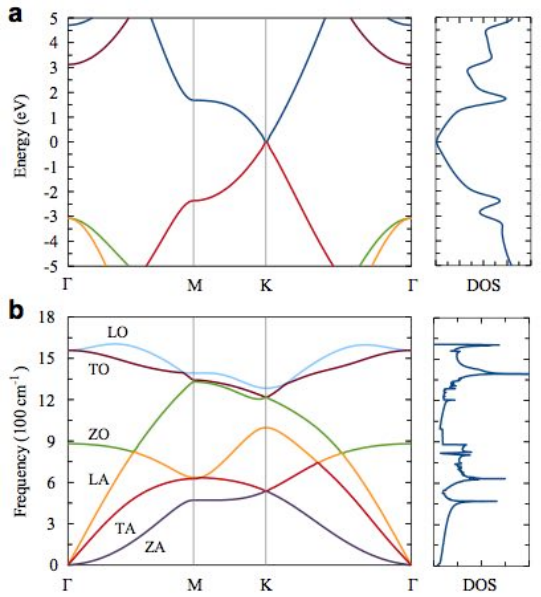
PART 1

MATERIAL DESIGN

QUANTUM ESPRESSO INTRODUCTION

TUTORIAL A-Z

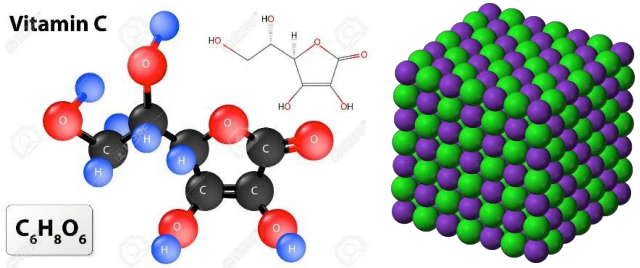
Design Material



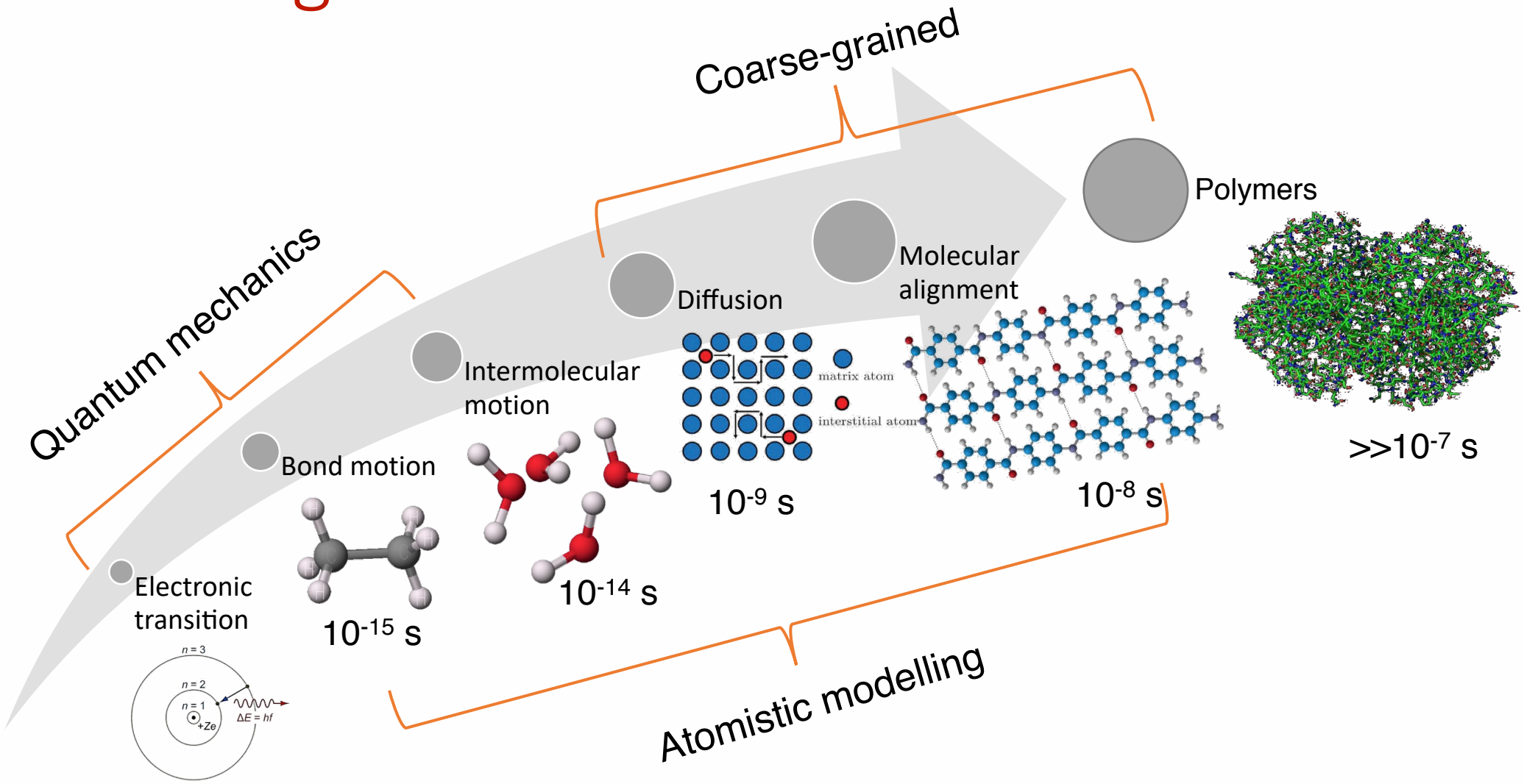
New structure prediction

Quantum simulation

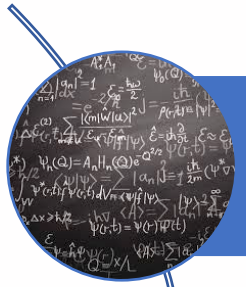
Properties analysis



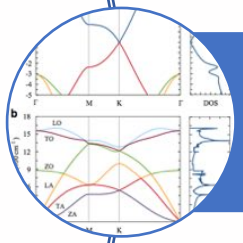
Time & length scale



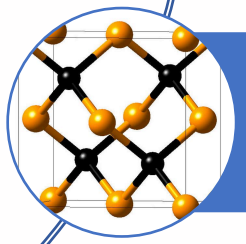
First-principles calculation



Based on quantum mechanics



Initially to calculate electronic structure



Now can predict the properties of materials

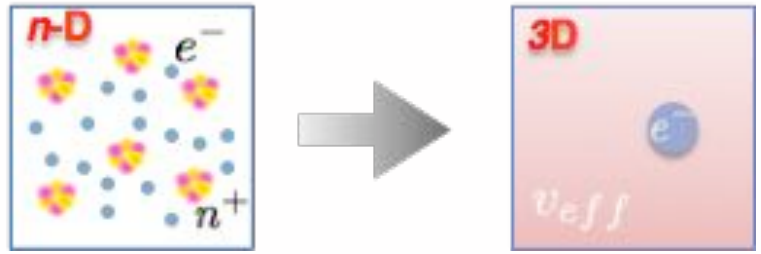
Solve Kohn-Sham equations

$$\left[-\frac{1}{2}\nabla^2 + V_{ion}(r) + V_H[n(r)] + V_{XC}[n(r)]\right]\psi_i(r) = \varepsilon_i\psi_i(r)$$

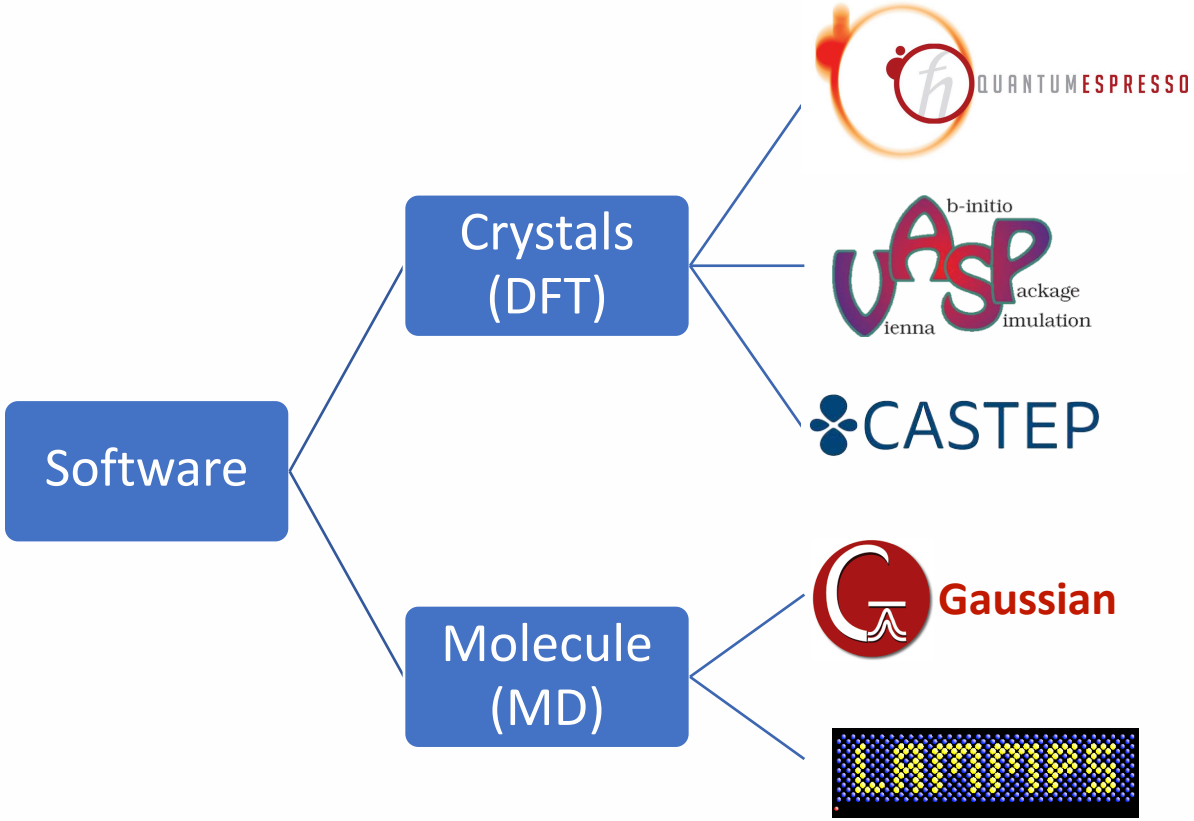
External nuclear potential

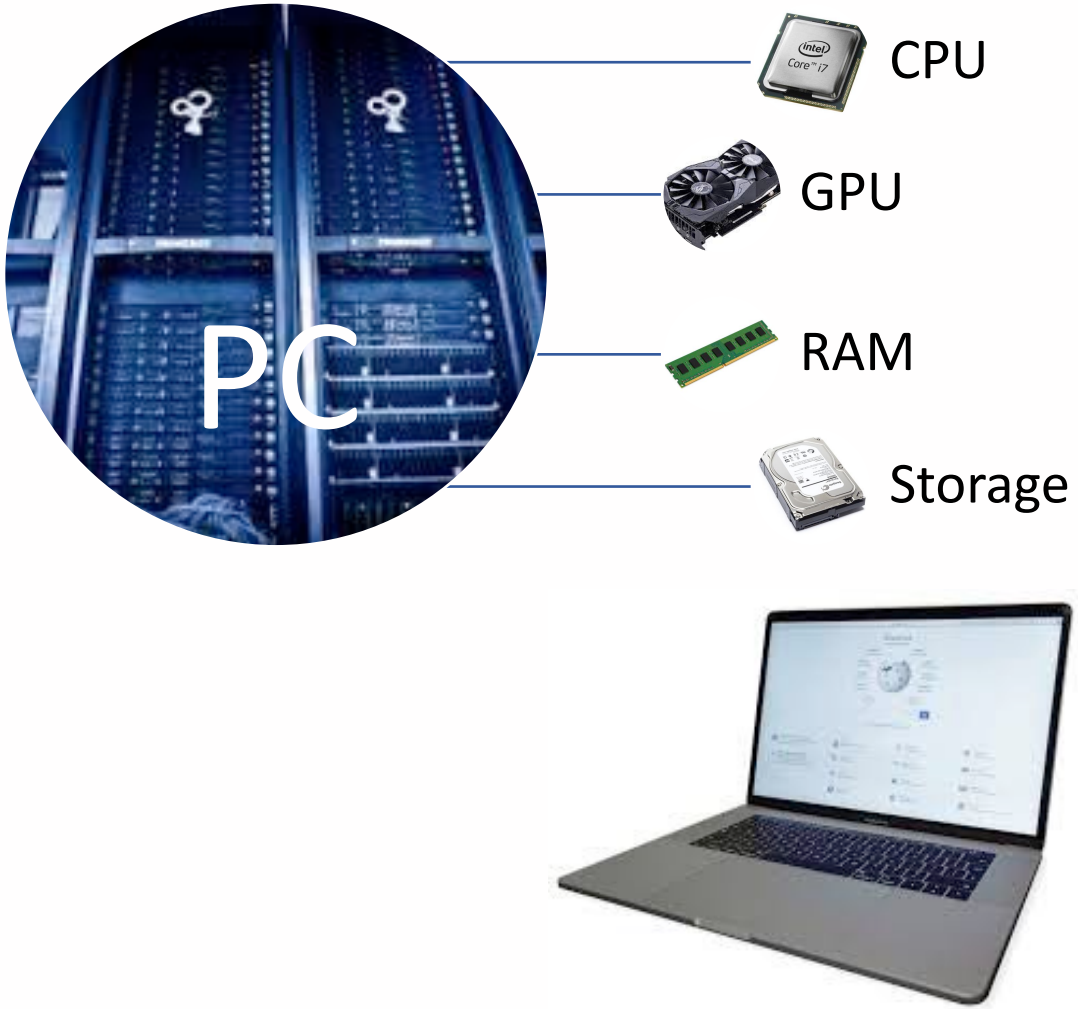
Hartree potential

Exchange-correlation potential



DFT tools


Software
Crystals (DFT)
Molecule (MD)
QUANTUMESPRESSO
b-initio
VASP
ienna
ackage
imulation
CASTEP
Gaussian
LAMMPS


PC
CPU
GPU
RAM
Storage