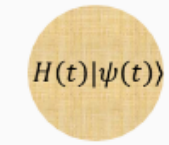
QUANTUMESPRESSO




QuantumNerd

YouTube

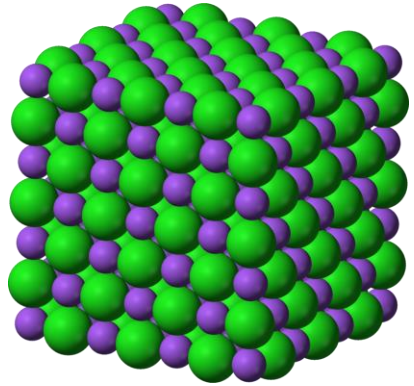
# Introduction

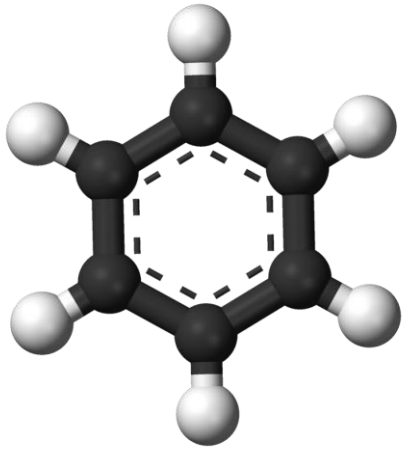
Quantum Espresso Tutorial 2019

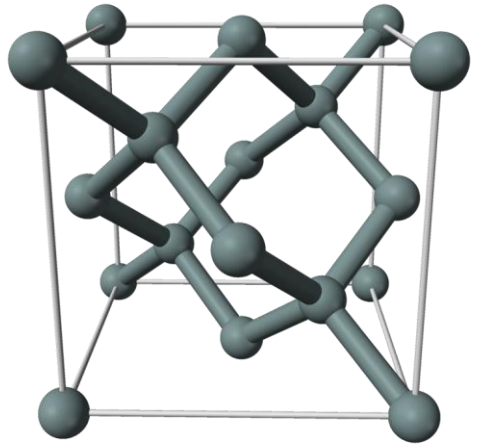
Quick start guide

# If you want to simulate…

- Material properties: band structure, DOS, absorption spectrum…
  - E.g. NaCl
- Structure of molecules, solid…
  - E.g. Benzene molecule, solid Si







QUANTUMESPRESSO

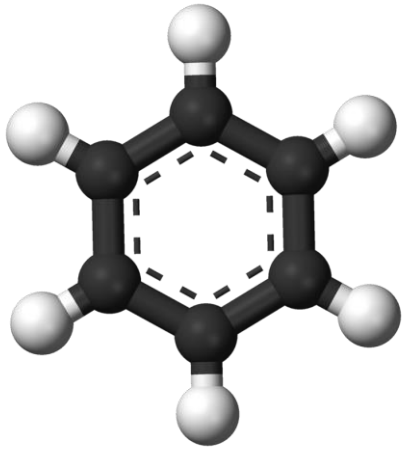

QuantumNerd

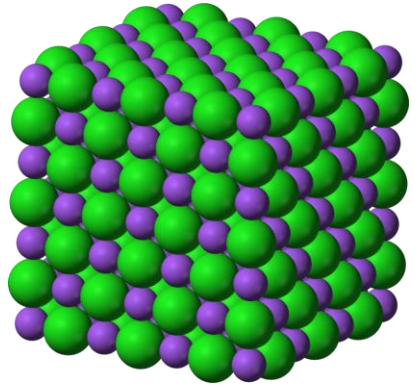
YouTube

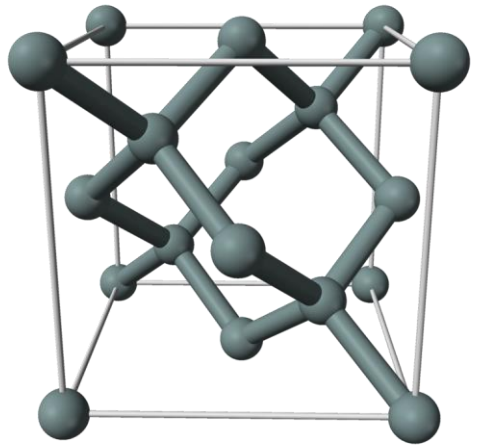
# If you want to simulate…

- Material properties: band structure, DOS, absorption spectrum…
  - E.g. NaCl
- Structure of molecules, solid…
  - E.g. Benzene molecule, solid Si

"Quantum mechanics"
"Quantum chemistry"







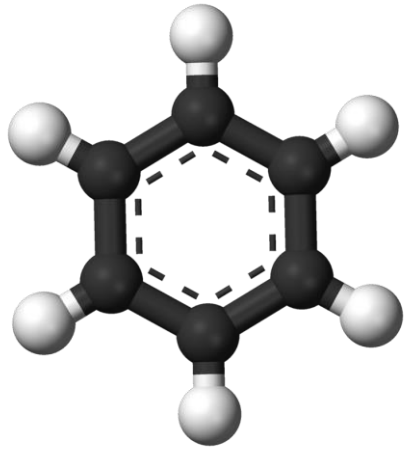
# If you want to simulate…

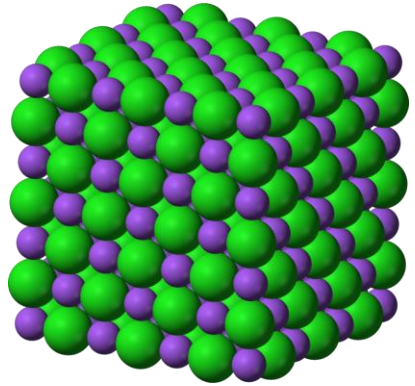
- Material properties: band structure, DOS, absorption spectrum…
  - E.g. NaCl
- Structure of molecules, solid…
  - E.g. Benzene molecule, solid Si

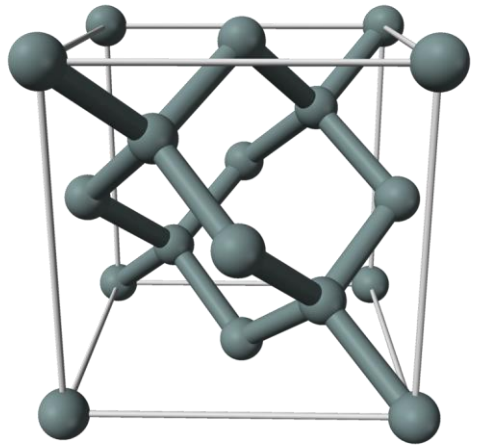
-> modern DFT softwares

"Quantum mechanics"
"Quantum chemistry"

Quantum Espresso










# DFT softwares

- Local basis set:
  - Gaussian
  - Orca
  - …
- Plain wave basis set:
  - VASP
  - WIEN2k
  - Quantum Espresso
  - …




# How to choose?

- Local basis set:
  - Gaussian
  - Orca
  - …

-> suitable for calculating molecules

- Plain wave basis set:
  - VASP
  - WIEN2k
  - Quantum Espresso
  - …

-> suitable for calculating periodic system, for example solids




# How to choose?

- Local basis set:
  - Gaussian
  - Orca
  - …

-> suitable for calculating molecules

- Plain wave basis set:
  - VASP
  - WIEN2k
  - Quantum Espresso
  - …

-> suitable for calculating periodic system, for example solids

-> what if molecule/addatom on the surface? Both…

QUANTUMESPRESSO

# How to choose?



- Local basis set: -> suitable for calculating molecules
  - Gaussian: commercial
  - Orca: free
  - …
- Plain wave basis set: -> suitable for calculating periodic system, for example solids
  - VASP: commercial, most widely used
  - WIEN2k: commercial. Less expensive than VASP
  - Quantum Espresso: free! Open source, also widely used
  - …

QUANTUMESPRESSO


QuantumNerd

YouTube

# Do commercial ones perform better?

- No!

Science Home News Journals Topics Careers

SHARE RESEARCH ARTICLE

## Reproducibility in density functional theory calculations of solids

Kurt Lejaeghere[1,*], Gustav Bihlmayer[2], Torbjörn Björkman[3,4], Peter Blaha[5], Stefan Blügel[2], Volker Blum[6], Damien Caliste[7,...]

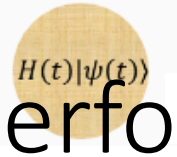
+ See all authors and affiliations

*Science* 25 Mar 2016:
Vol. 351, Issue 6280, aad3000
DOI: 10.1126/science.aad3000

Lejaeghere, Kurt, et al. "Reproducibility in density functional theory calculations of solids." *Science* 351.6280 (2016): aad3000.

| | | average <Δ> | AE | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | Elk | exciting | FHI-aims/tier2 | FLEUR | FPLO/T+F+s | RSPt | WIEN2k/acc |
| PAW | GBRV12/ABINIT | 0.9 | 0.9 | 0.8 | 0.8 | 0.9 | 1.3 | 1.1 | 0.8 |
| | GPAW09/ABINIT | 1.4 | 1.3 | 1.3 | 1.3 | 1.3 | 1.7 | 1.5 | 1.3 |
| | GPAW09/GPAW | 1.6 | 1.5 | 1.5 | 1.5 | 1.5 | 1.8 | 1.7 | 1.5 |
| | JTH02/ABINIT | 0.6 | 0.6 | 0.6 | 0.6 | 0.6 | 0.9 | 0.7 | 0.5 |
| | PSlib100/QE | 0.9 | 0.9 | 0.8 | 0.8 | 0.8 | 1.3 | 1.1 | 0.8 |
| | VASPGW2015/VASP | 0.6 | 0.4 | 0.4 | 0.4 | 0.6 | 1.0 | 0.8 | 0.3 |
| USPP | GBRV14/CASTEP | 1.1 | 1.1 | 1.1 | 1.0 | 1.0 | 1.4 | 1.3 | 1.0 |
| | GBRV14/QE | 1.1 | 1.0 | 1.0 | 0.9 | 1.0 | 1.4 | 1.3 | 1.0 |
| | OTFG9/CASTEP | 0.7 | 0.4 | 0.5 | 0.5 | 0.7 | 1.0 | 1.0 | 0.5 |
| | SSSP/QE | 0.5 | 0.4 | 0.3 | 0.3 | 0.5 | 0.9 | 0.8 | 0.3 |
| | Vdb2/DACAPO | 6.3 | 6.3 | 6.3 | 6.3 | 6.3 | 6.4 | 6.5 | 6.2 |
| NCPP | FHI98pp/ABINIT | 13.3 | 13.5 | 13.4 | 13.4 | 13.2 | 13.0 | 13.2 | 13.4 |
| | HGH/ABINIT | 2.2 | 2.2 | 2.2 | 2.2 | 2.0 | 2.3 | 2.2 | 2.1 |
| | HGH-NLCC/BigDFT | 1.1 | 1.1 | 1.1 | 1.1 | 1.0 | 1.2 | 1.1 | 1.0 |
| | MBK2013/OpenMX | 2.0 | 2.1 | 2.1 | 2.1 | 1.9 | 1.8 | 1.8 | 2.0 |
| | ONCVPSP(PD0.1)/ABINIT | 0.7 | 0.7 | 0.7 | 0.7 | 0.6 | 1.0 | 0.8 | 0.6 |
| | ONCVPSP(SG15)1/QE | 1.4 | 1.4 | 1.3 | 1.3 | 1.3 | 1.6 | 1.5 | 1.3 |
| | ONCVPSP(SG15)2/CASTEP | 1.4 | 1.4 | 1.4 | 1.4 | 1.3 | 1.6 | 1.5 | 1.4 |

QUANTUMESPRESSO



QuantumNerd

YouTube

# Do commercial ones perform better?

- No!

Science Home News Journals Topics Careers

SHARE RESEARCH ARTICLE

## Reproducibility in density functional theory calculations of solids

Kurt Lejaeghere[1,*], Gustav Bihlmayer[2], Torbjörn Björkman[3,4], Peter Blaha[5], Stefan Blügel[2], Volker Blum[6], Damien Caliste[7,...]
+ See all authors and affiliations

*Science* 25 Mar 2016:
Vol. 351, Issue 6280, aad3000
DOI: 10.1126/science.aad3000

| | | average <Δ> | AE | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | Elk | exciting | FHI-aims/tier2 | FLEUR | FPLO/T+F+s | RSPt | WIEN2k/acc |
| PAW | GBRV12/ABINIT | 0.9 | 0.9 | 0.8 | 0.8 | 0.9 | 1.3 | 1.1 | 0.8 |
| | GPAW09/ABINIT | 1.4 | 1.3 | 1.3 | 1.3 | 1.3 | 1.7 | 1.5 | 1.3 |
| | GPAW09/GPAW | 1.6 | 1.5 | 1.5 | 1.5 | 1.5 | 1.8 | 1.7 | 1.5 |
| | JTH02/ABINIT | 0.6 | 0.6 | 0.6 | 0.6 | 0.6 | 0.9 | 0.7 | 0.5 |
| | PSlib100/QE | 0.9 | 0.9 | 0.8 | 0.8 | 0.8 | 1.3 | 1.1 | 0.8 |
| | VASPGW2015/VASP | 0.6 | 0.4 | 0.4 | 0.4 | 0.6 | 1.0 | 0.8 | 0.3 |
| USPP | GBRV14/CASTEP | 1.1 | 1.1 | 1.1 | 1.0 | 1.0 | 1.4 | 1.3 | 1.0 |
| | GBRV14/QE | 1.1 | 1.0 | 1.0 | 0.9 | 1.0 | 1.4 | 1.3 | 1.0 |
| | OTFG9/CASTEP | 0.7 | 0.4 | 0.5 | 0.5 | 0.7 | 1.0 | 1.0 | 0.5 |
| | SSSP/QE | 0.5 | 0.4 | 0.3 | 0.3 | 0.5 | 0.9 | 0.8 | 0.3 |
| | Vdb2/DACAPO | 6.3 | 6.3 | 6.3 | 6.3 | 6.3 | 6.4 | 6.5 | 6.2 |
| NCPP | FHI98pp/ABINIT | 13.3 | 13.5 | 13.4 | 13.4 | 13.2 | 13.0 | 13.2 | 13.4 |
| | HGH/ABINIT | 2.2 | 2.2 | 2.2 | 2.2 | 2.0 | 2.3 | 2.2 | 2.1 |
| | HGH-NLCC/BigDFT | 1.1 | 1.1 | 1.1 | 1.1 | 1.0 | 1.2 | 1.1 | 1.0 |
| | MBK2013/OpenMX | 2.0 | 2.1 | 2.1 | 2.1 | 1.9 | 1.8 | 1.8 | 2.0 |
| | ONCVPSP(PD0.1)/ABINIT | 0.7 | 0.7 | 0.7 | 0.7 | 0.6 | 1.0 | 0.8 | 0.6 |
| | ONCVPSP(SG15)1/QE | 1.4 | 1.4 | 1.3 | 1.3 | 1.3 | 1.6 | 1.5 | 1.3 |
| | ONCVPSP(SG15)2/CASTEP | 1.4 | 1.4 | 1.4 | 1.4 | 1.3 | 1.6 | 1.5 | 1.4 |

Lejaeghere, Kurt, et al. "Reproducibility in density functional theory calculations of solids." *Science* 351.6280 (2016): aad3000.




# Do commercial ones perform better?

- VASP:
  - expensive license
  - offers well-maintained pseudopotential library
- Quantum Espresso:
  - free, open source
  - updated and maintained well
  - many open-source pseudopotential library available, covering nearly all elements. But you may not find one if you have specific requirement




# Summary

- “Quantum chemistry”
- DFT softwares
- Local basis set v.s. plain wave basis set
- VASP v.s. Quantum Espresso




# Later

- Quick start guide:
  - System requirements
  - Download
  - Installation: most difficult part of using Quantum Espresso
  - Basic examples
- More projects