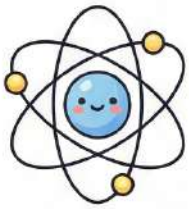
MY FIRST COMPUTATIONAL CHEMISTRY ALPHABET



A a - Atom

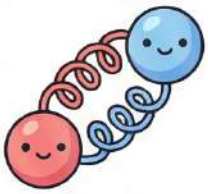
B b - Basis set

C c - Contour plot

D d - Density plot

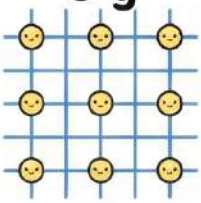
E e - Energy surface

F f



F - Force field

G g



Grid

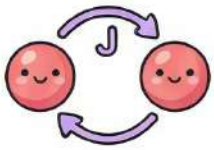
H h

H - Hamiltonian matrix

I i

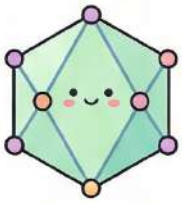
I - Isosurface

J j



J-coupling

K k

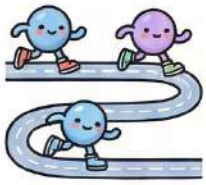


k-space

L l

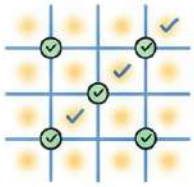
LUMO

M m



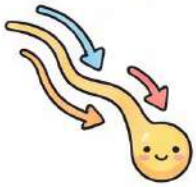
Molecular dynamics

N n



Numerical integration

O o



Optimization path

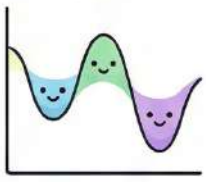
P p

Potential energy curve

Q q

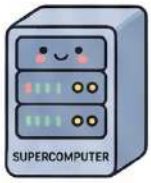
Quantum wavefunction

R r



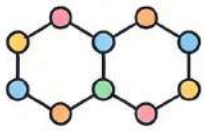
Reaction coordinate diagram

S s



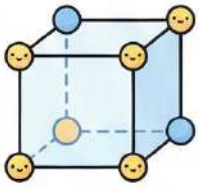
Supercomputer

T t



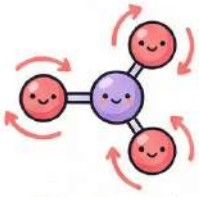
Tight-binding model

U u



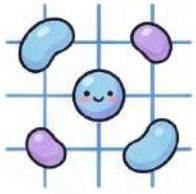
Unit cell

V v



Vibrational mode

W w

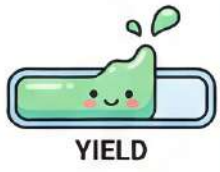


Wannier functions

X x

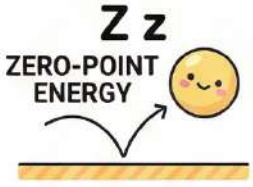
XTB

Y y



Yield

Z z



Zero-point energy