

# Computational Nanomaterial: From Semiconductor to Low-dimensional Materials

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# The Nobel Prize in Chemi

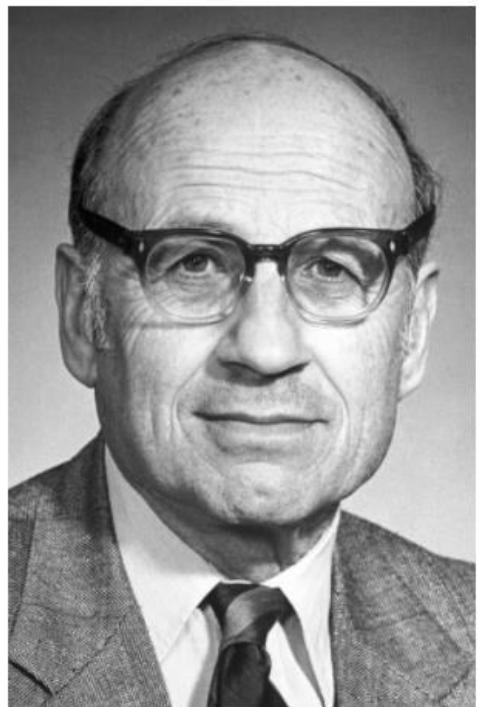


Photo from the Nobel Foundation archive.

Walter Kohn

Prize share: 1/2

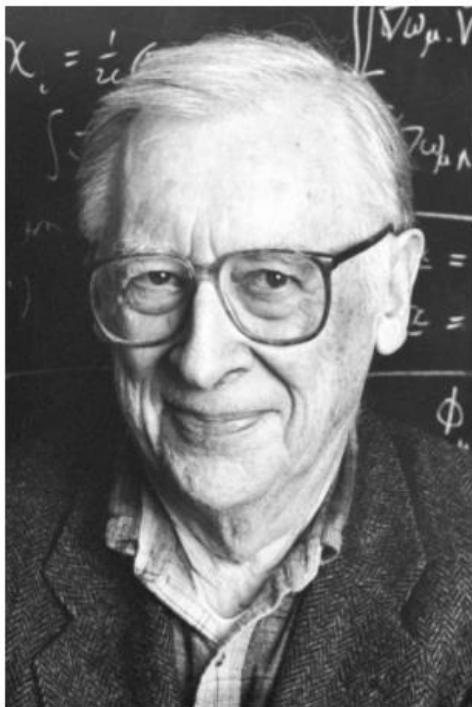


Photo from the Nobel Foundation archive.

John A. Pople

Prize share: 1/2

## Gaussian 92

### Major New Features:

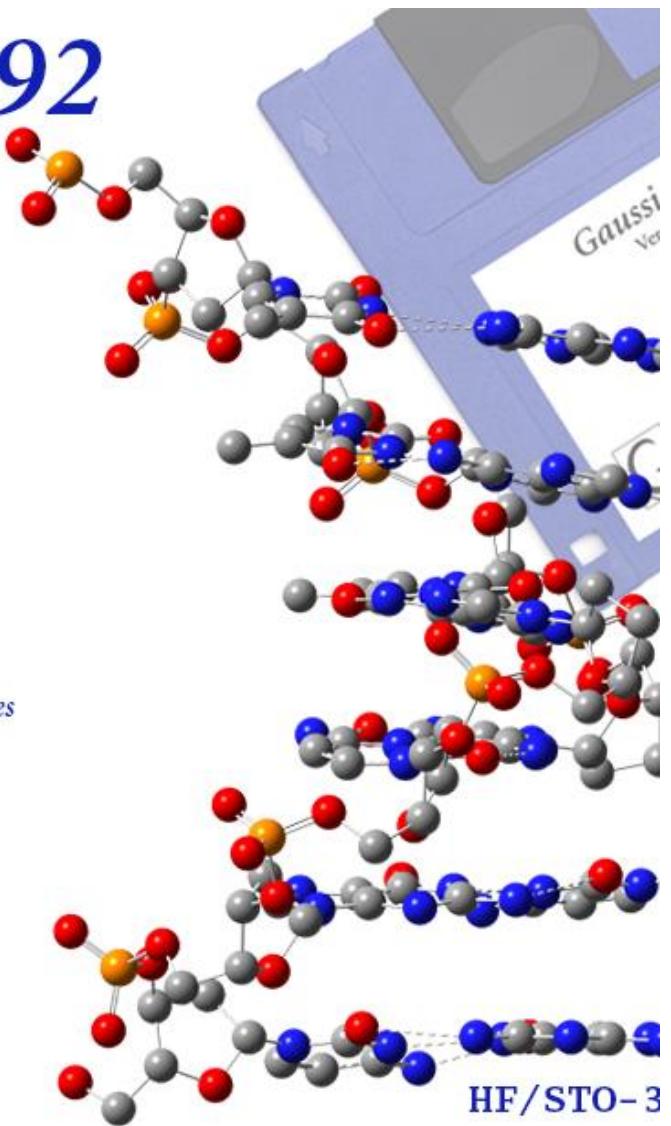
- ◆ Electrostatic potentials
- ◆ MP2 frequencies
- ◆ Onsager solvation model
- ◆ Gaussian 92/DFT
- ◆ Pure & hybrid density functional model chemistries

### Performance Enhancements:

- ◆ Automated direct/semi-direct SCF

### Challenging Calculation:

- ◆ DNA 6-mer energy & atomic charges



## Quantum-mechanics

In quantum mechanics, a system is presented by Schrodinger equation

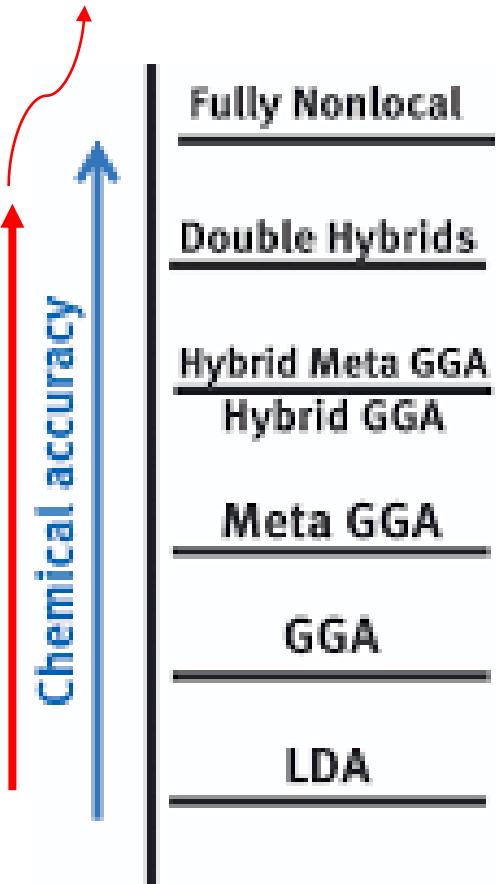
$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi = E\Psi.$$

For many-body problems:

$$\hat{H}\Psi(r_1, \dots, r_n, R_1, \dots, R_N) = E\Psi(r_1, \dots, r_n, R_1, \dots, R_N),$$

## Exchange Correlation

Computational cost



B2PLYP, B2GP -PLYP, DSD -PBEP86

B1B95, BB1K, PBE1KCIS  
B3LYP, B3P86, B3PW91, BH&LYP

BB95, MPW1K, TPSS, VSXC

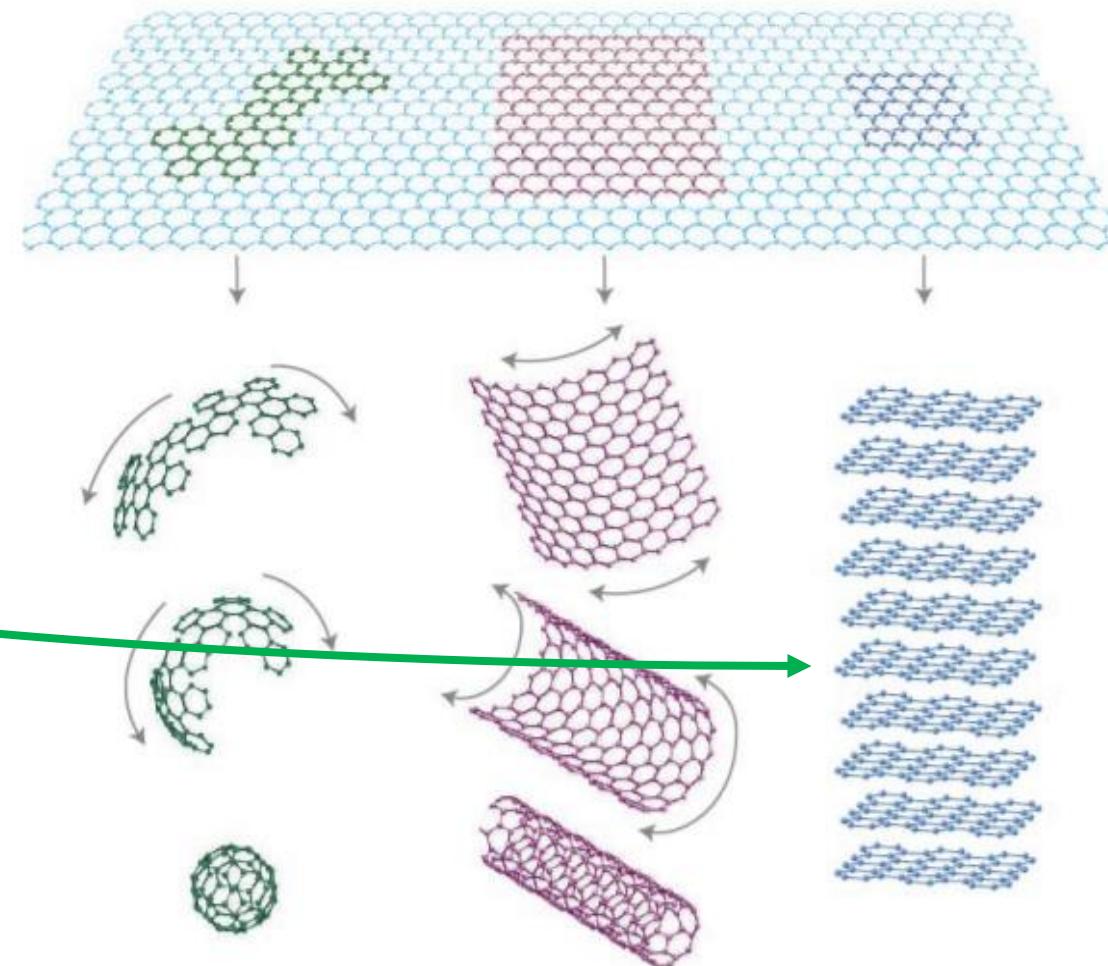
BLYP, BP86, BPW91, G96LYP,  
HCTC, OLYP, PBE

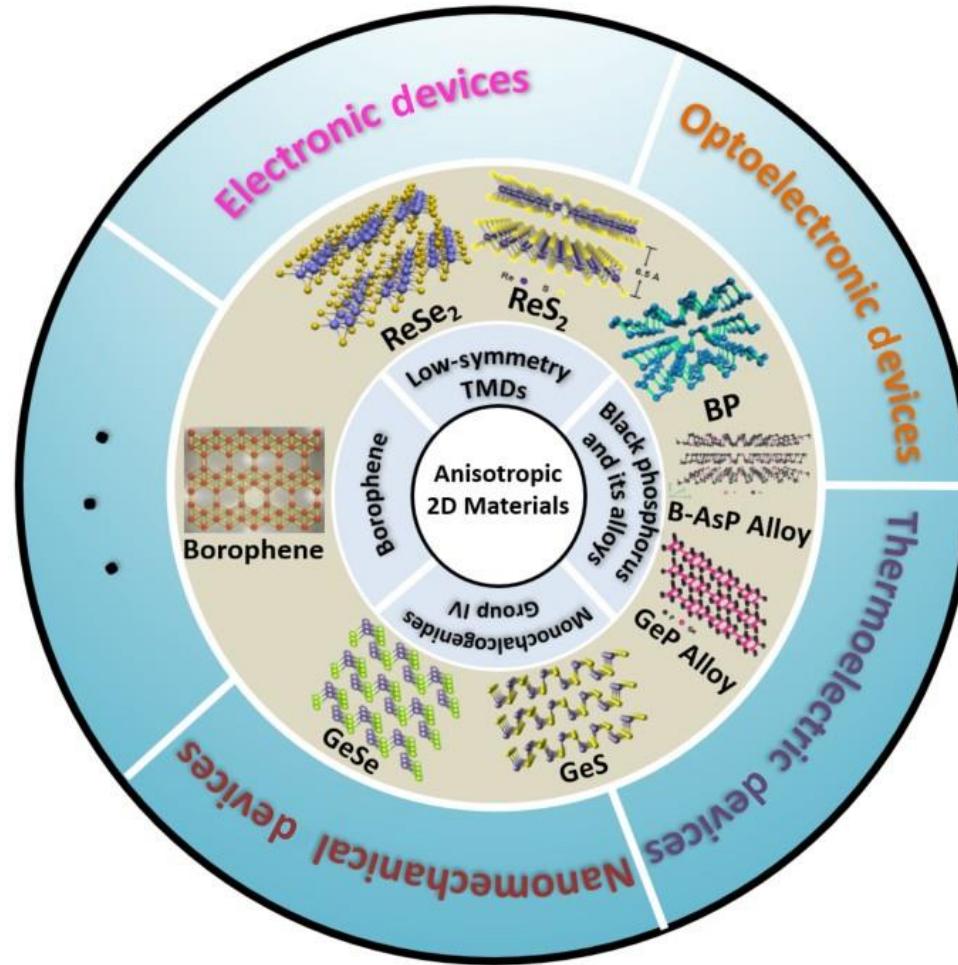
SPWL

# Nanomaterials Modeling

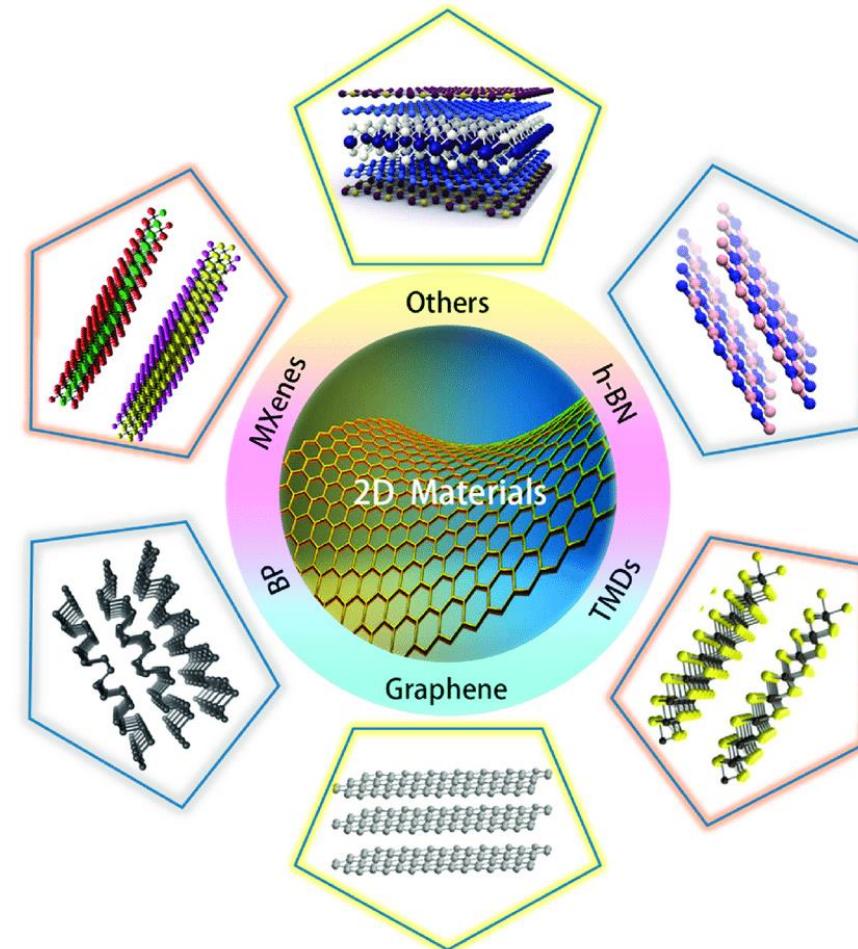


Novoselov et al. Science 306, 666 (2004)



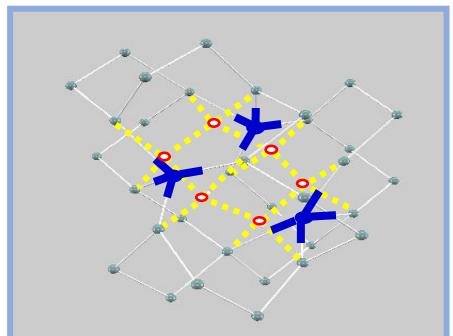


Dong, et al. Molecules 2019, 24(1), 88

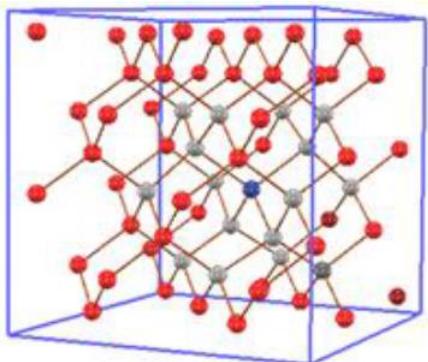


Zhao et al. Nano Res. 14, 897–919 (2021)

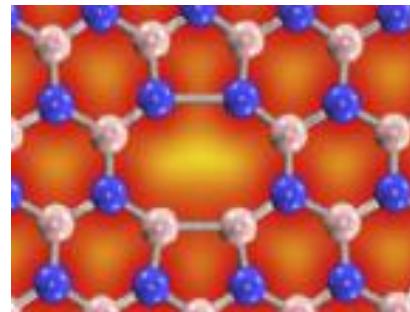
## 2D and 3D Defective Materials



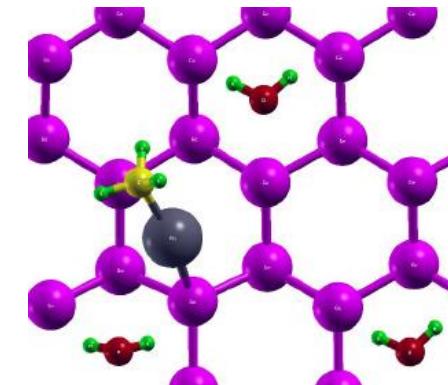
3D Si/Ge



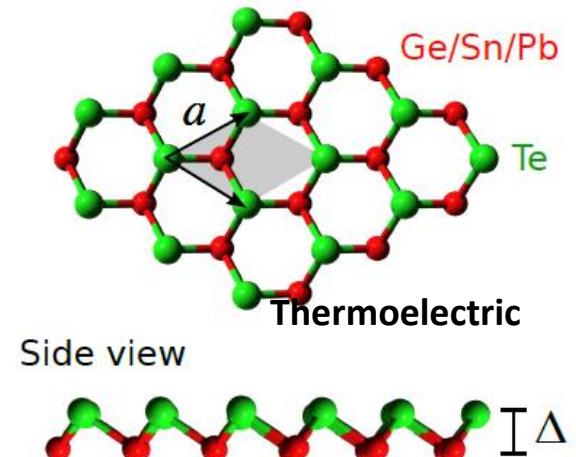
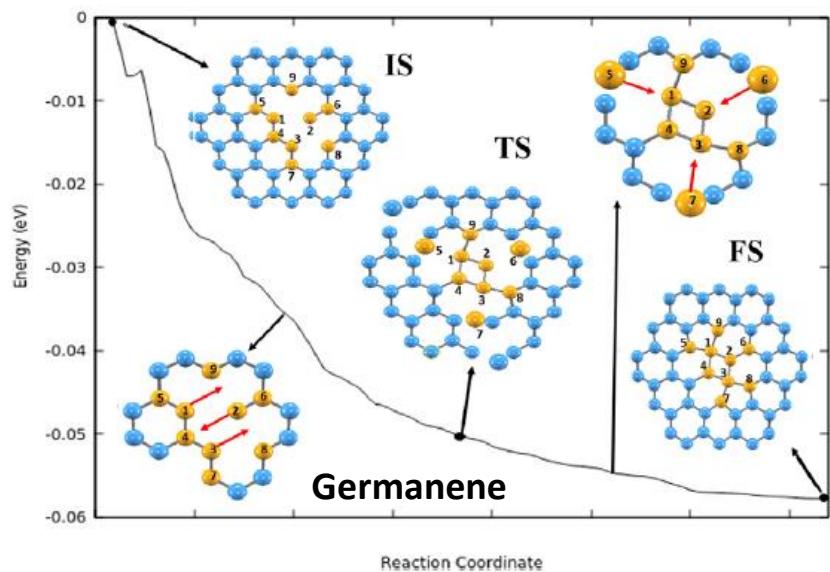
NV-Diamond



2D h-BN



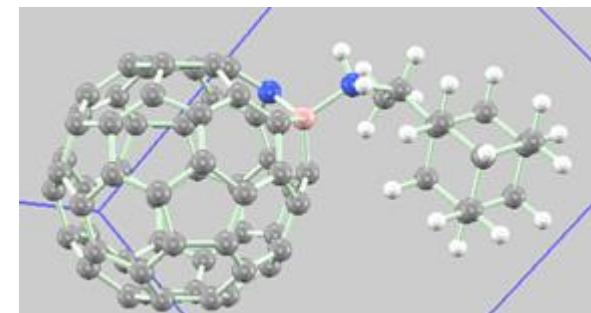
Germanene-Methylmercury



Side view



Collaborators: Dr. Ari Dwi Nugraheni | Dr. Iman Santoso | Dr. Pekik Nurwantoro | Dr. Moh. Adhib U. A. | Dr. Sasfan A. W. (BRIN) | Dr. Nadya Amalia (BRIN)



Drug delivery application

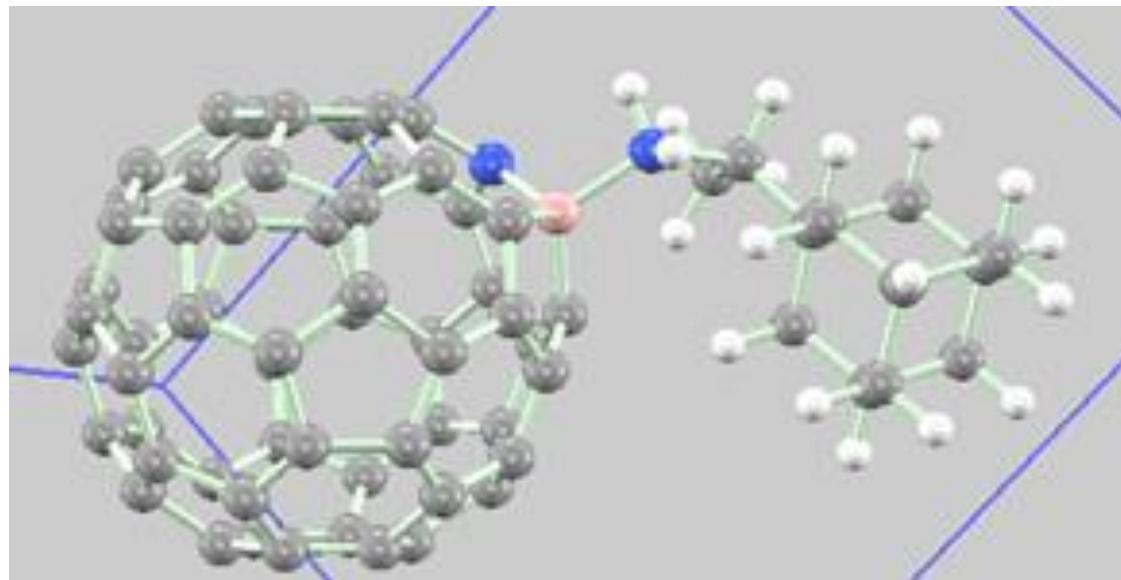
# Topik S1 dan S2

- Interaction between Fullerene dan drug molecule – drug delivery application
- Interaction between Fullerene /Nanoparticle dan nucleobases – gene delivery application
- Phonon simulation for defective semiconductor
- 2D material for thermoelectric



# Topik S1 dan S2

- Interaction between Fullerene dan drug molecule – drug delivery application



# Topik S1 dan S2

- Interaction between Fullerene/Nanoparticle dan nucleobases – gene delivery application

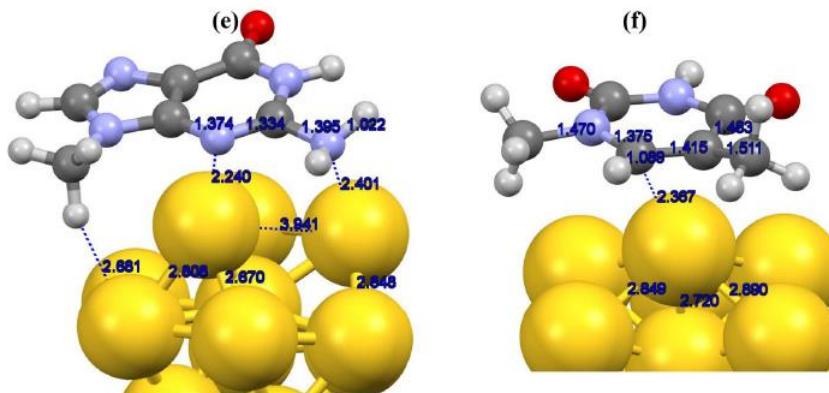
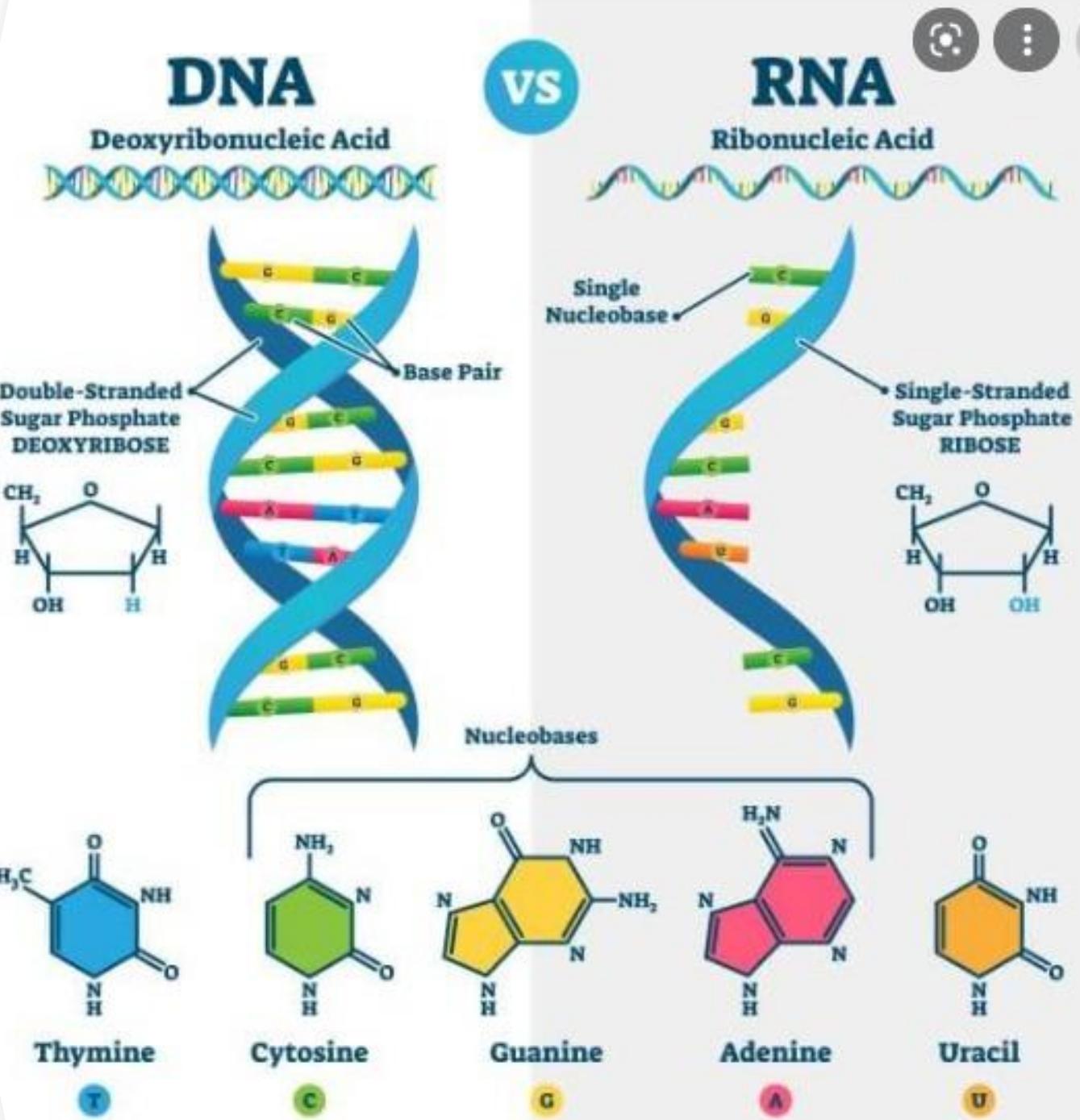


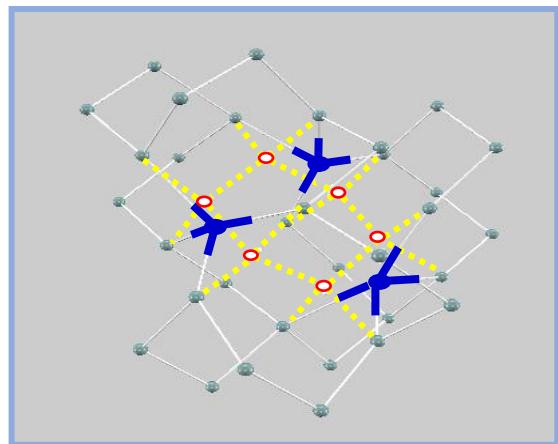
Figure 2. Representation of potential active sites for (a) Au13 cluster and (b) adenine. Optimized structures of (c) adenine/Au13, (d) cytosine/Au13, (e) guanine/Au13, and (f) thymine/Au13 complexes with DFT-D3/TZVP and implicit solvent media.

<https://doi.org/10.1038/s41598-020-80161-z>

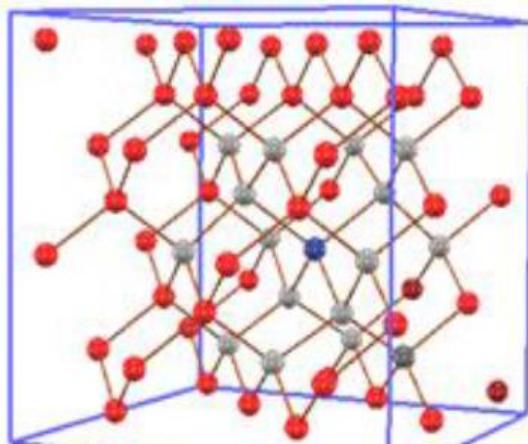


# Topik S1 dan S2

- Phonon simulation for defective semiconductor



3D Si/Ge

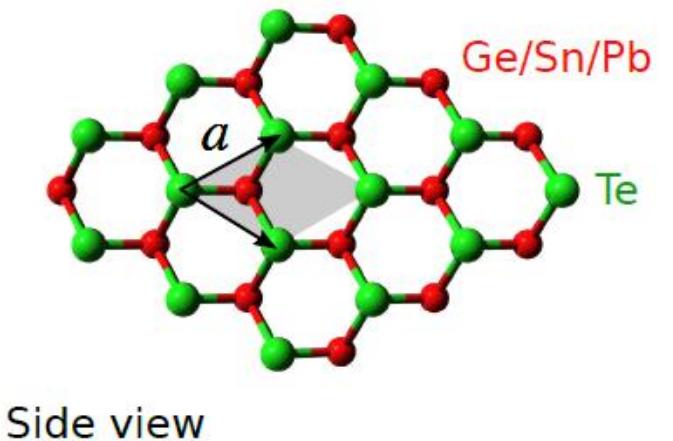


NV-Diamond



# Topik S1 dan S2

➤ 2D material for thermoelectric



Side view

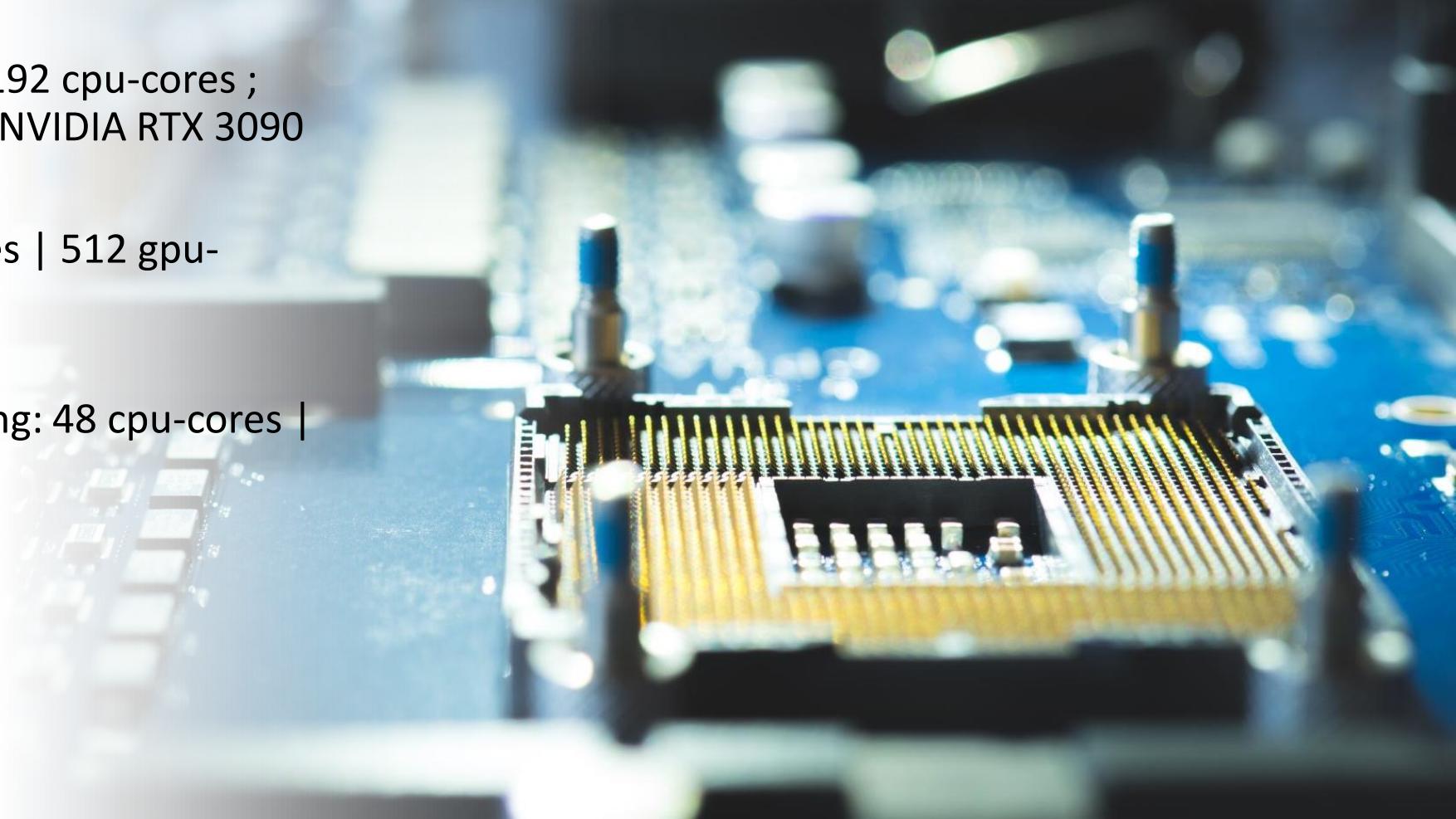


Thermoelectric



# Fasilitas Komputasi

- Supercomputer Efison (192 cpu-cores ;  
2384 Threads | 3 x GPU NVIDIA RTX 3090)
- Jetson Xavier (8 cpu-cores | 512 gpu-cores)
- P-HPC Optimetri (on-going: 48 cpu-cores |  
768 gpu-cores)



**ACCELERATING RESEARCH AND SCIENTIFIC DISCOVERY WITH HIGH PERFORMANCE COMPUTING**  
POWERED BY AMD EPYC

**EFISON**

**Dr.Sc. Sholihun, S.Si., M.S**  
Universitas Gadjah Mada

Bidang Fisika Kuantum  
Software: PHASE0, Quantum ESPRE

*Quantum-mechanical-based Simulations  
Semiconductor Materials*

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Penelitian nanomaterial dengan komputasi DFT (untuk menguji the stability of multivacancies pad

**Wilson Lisan**  
CEO of Efison Lisan Teknologi

**EFISON**

**ALELEON**  
SUPERCOMPUTER

**EUREKA!**  
Program Sponsorship Superkomputer EFISON

**Periode 1**

## Spesifikasi Utama

Hardware - HPC Aleleon Mk.II per April 2021

Komponen	Jumlah	Spesifikasi	Nama Partisi Kluster Hardware
Compute Node CPU	3	AMD EPYC Rome 64 cores / 128 threads, RAM 256GB. <b>Total</b> 192 cores / 384 threads, RAM 768GB	<b>epyc</b>
Compute Node GPU	1	AMD TR 64 core / 128 thread, 2x GPU NVIDIA RTX 3090	<b>gpu_ampere</b>
Storage HOME	1	20 TB RAID-10, terpusat	
High-speed network	1	100 GbE RDMA/RoCE, QSFP28 Mellanox	
Data network	1	10 GbE SFP+	

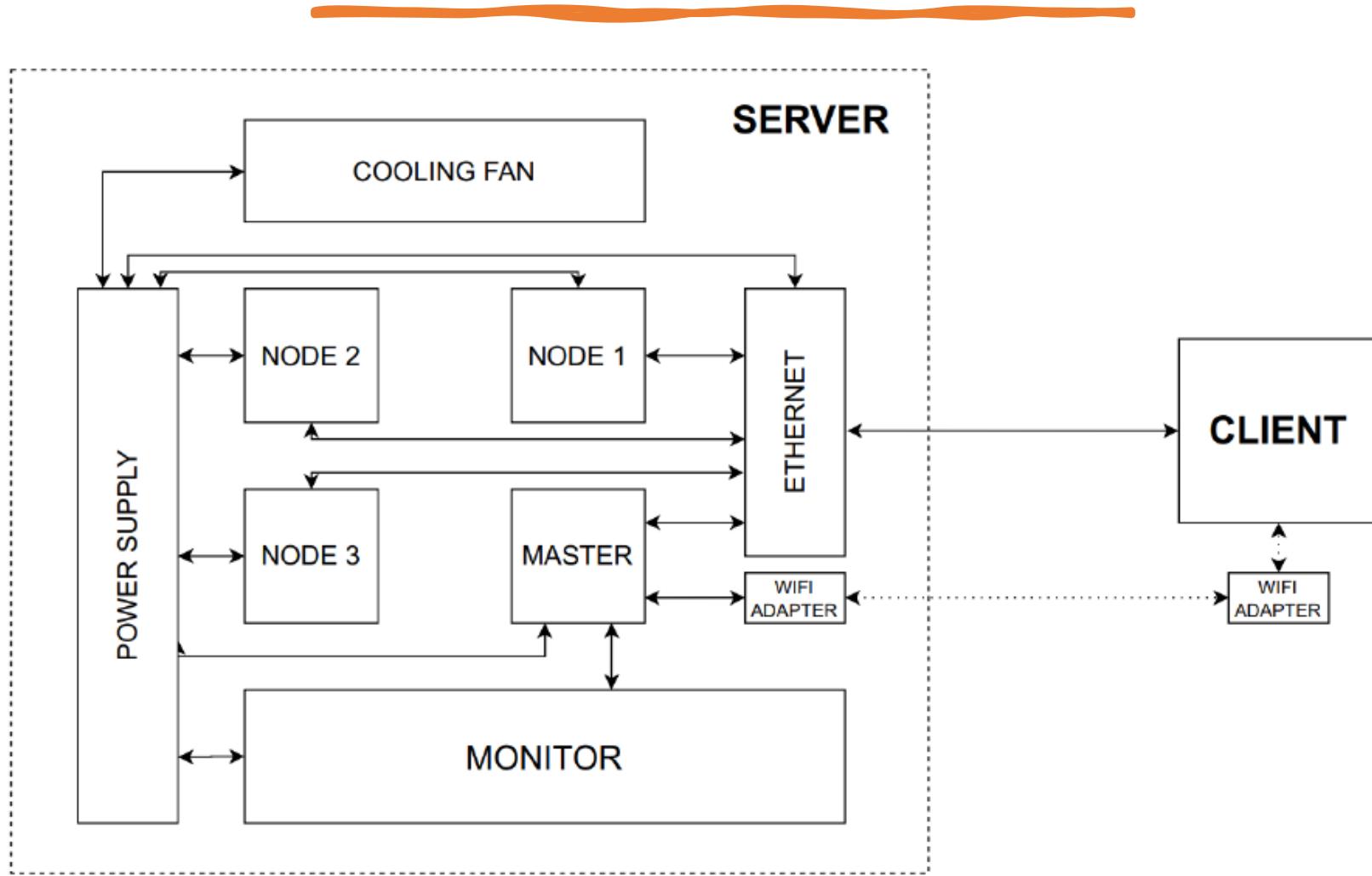


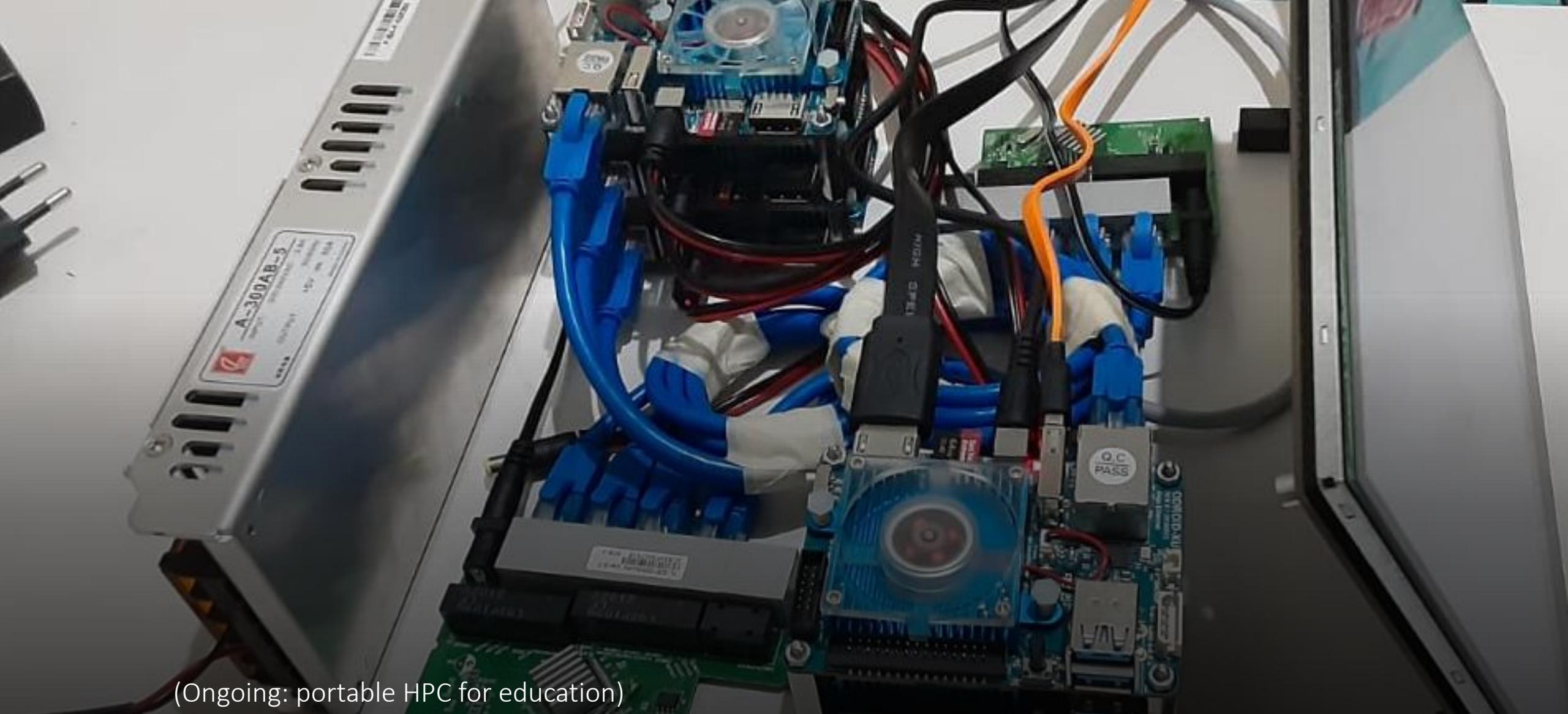
HPC Aleleon Mk.II dengan bangga menggunakan ASUS HPC



# Pra-StartUp OPTIMETRI

(Ongoing: portable HPC for education)





(Ongoing: portable HPC for education)

**Pra-StartUp OPTIMETRI**

# Pemrograman dan Komputasi Numerik Menggunakan Python

<https://ugmpress.ugm.ac.id/id/product/fisika/pemrograman-dan-komputasi-numerik-menggunakan-python>

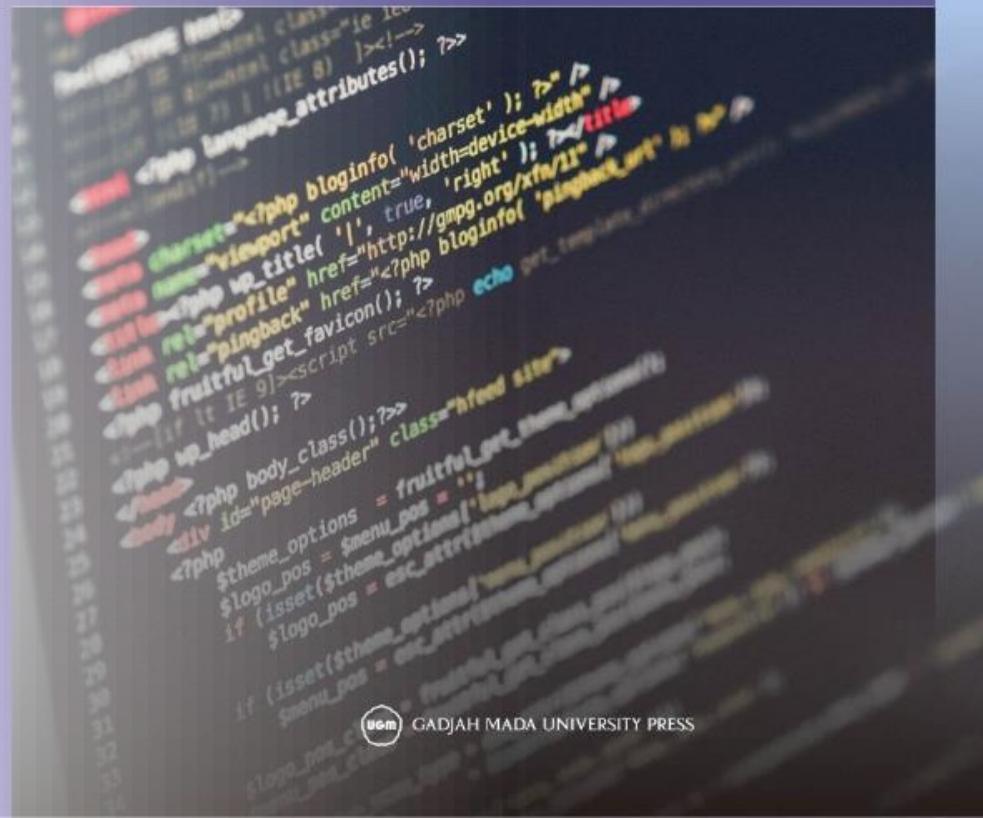
Buku ini bertujuan untuk membantu mahasiswa dalam belajar pemrograman Python dan Komputasi Numerik. Mengingat pentingnya peran komputasi numerik dalam kehidupan sehari-hari, buku ini diawali dengan penjelasan tentang *what is programming*. Motivasi pemilihan bahasa pemrograman Python yang bersifat *open source*, kualitas kode yang *powerfull* (memiliki fungsi-fungsi yang lengkap), *multi-platform programming*, dan *cross-platform* (dapat dijalankan pada berbagai sistem operasi).

Buku ini dibuat dengan tujuan agar selain menjadi buku ajar, buku ini juga dapat membantu para pembaca yang ingin belajar pemrograman Python, baik secara autodidak maupun dengan bantuan dosen. Semoga buku ini diharapkan pembaca dapat memahami konsep pemrograman dan metode numerik dan dapat menerapkan pengetahuan tersebut untuk menyelesaikan permasalahan pada bidang fisika, teknologi, teknik, material, dan lainnya.

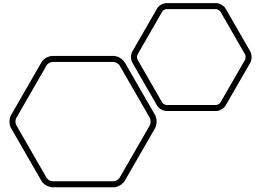
ISBN 978-623-95212-0-0  
Penerjemah: Dr. H. Sholihun, M.Si  
Penulis: Sholihun & Zohan Syah Fatomi



Pemrograman dan Komputasi Numerik Menggunakan Python



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# TERIMAKASIH