

8th African School on Electronic Structure Methods and Applications - ASESMA 2025 (smr 4081)

9-20 June 2025 Accra - Ghana

WEEK 1 : BASIC SESSION

Monday, June 9 (Day 1)

08:00 Registration formalities 30' |

Venue: forecourt of School of Physical and Mathematical Sciences

08:30 Welcome & Introduction 30'

Directors of the school (Garu, Richard, Shobhana, Nicola, Omolulu, Martin, Krishna, Nana Ama)

09:00 Introduction to DFT and Kohn-Sham equation 1h

Speaker: Richard Martin

10:00 Coffee Break 30'

10:30 Crystals and band structures 1h

Speaker: Javier Junquera

11:30 Open discussion session 1h

Speaker: Shobhana Narasimhan

12:30 Lunch Break 1h30'

14:00 Hands-on: Intro to Linux (Unix commands), Xmgrace, Xcrysden, DFT codes overview, etc. 2h

Speaker: George Manyali / James Sifuna / Nelson Dzade / Maram Ali Ahmed Musa / Omamuyovwi Rita Jolayemi / Fatema Mohamed / Alberto Carta

16:00 Poster session 2h

20:00 Evening session 1h

Speaker: Shobhana Narasimhan

Tuesday, June 10 (Day 2)

08:30 Speeches by ministers and diplomats 1h30' |

Venue: Conference Hall of WACCBIP

Officials of the University - Vice Chancellor, Provost, College of Basic and Applied Sciences | *Vice-Chancellor or Representative to Chair*

Diplomatic envoys

CEO of Minerals Commission, CEO of Environmental Protection Agency and

Directors of supporting organisations

(Ministers of State – Ministry of Education, Ministry of Environment, Science and Technology, Ministry of Energy and Green Transition)

Members of Parliament

[Richard Martin: ASESMA](#)

10:00 Coffee Break 30'

10:30 Basis sets (Plane waves, localized basis set, ...) 1h

Speaker: [Michele Pavanello](#)

11:30 k-point sampling 1h

Speaker: [Shobhana Narasimhan](#)

12:30 Lunch Break 1h30'

14:00 Discussion: Q&A

14:30 Hands-on: Total energy, cutoff, k points, convergence, DOS, (molecules, semiconductors (2D, 3D)) 1h30'

Speaker: [Chiara Cignarella](#) / [George Manyali](#) / [James Sifuna](#) / [Nelson Dzade](#) / [Maram Ali Ahmed Musa](#) / [Omamuyovwi Rita Jolayemi](#)

16:00 Coffee Break 30'

16:30 Hands-on: Total energy, cutoff, k points, convergence, DOS, (molecules, semiconductors (2D, 3D)) 1h30'

Speaker: [Chiara Cignarella](#) / [George Manyali](#) / [James Sifuna](#) / [Nelson Dzade](#) / [Maram Ali Ahmed Musa](#) / [Omamuyovwi Rita Jolayemi](#)

20:00 Evening session 1h

Speaker: [Nithaya Chetty](#) "History of ASESMA"

Wednesday, June 11 (Day 3)

09:00 Metals and smearing techniques 1h

Speaker: TBD

10:00 Pseudopotentials 1h

Speaker: [Javier Junquera](#) & [Nelson Dzade](#)

11:00 Coffee Break 30'

11:30 Exchange-correlation functionals (LDA and GGA) 1h

Speaker: [Omololu Akin-Ojo](#)

12:30 Lunch Break 1h30'

14:00 Discussion: Q&A

14:30 Hands-on: Smearing, bandstructure, xc functionals 1h30'

Speaker: [Omamuyovwi Rita Jolayem](#) / [George Manyali](#) / [James Sifuna](#) / [Nelson Dzade](#) / [Maram Ali Ahmed Musa](#) / [Chiara Cignarella](#) / [Alberto Carta](#)

16:00 Coffee Break 30'

16:30 Hands-on: Smearing, bandstructure, xc functionals 1h30'

Speaker: [Omamuyovwi Rita Jolayem](#) / [George Manyali](#) / [James Sifuna](#) / [Nelson Dzade](#) / [Maram Ali Ahmed Musa](#) / [Chiara Cignarella](#) / [Alberto Carta](#)

20:00 Evening session 1h

Speaker: TBD

Thursday, June 12 (Day 4)

09:00 Forces and relaxations 1h

Speaker: [Nicola Seriani](#)

10:00 Lattice Dynamics: From Phonons to Thermodynamics 30'

Speaker: [Christian Carbogno](#)

10:30 Coffee Break 30'

11:00 Lattice Dynamics: From Phonons to Thermodynamics - continuation 1h30'

Speaker: [Christian Carbogno](#)

12:30 Lunch Break 1h30'

14:00 Discussion: Q&A

14:30 Hands-on: Forces, relaxation 1h30'

Speaker: [Alberto Carta](#) / [Chiara Cignarella](#) / [Nelson Dzade](#) / [George Manyali](#) / [James Sifuna](#) / [Omamuyovwi Rita Jolayem](#) / [Maram Ali Ahmed Musa](#)

16:00 Coffee Break 30'

16:30 Hands-on: phonons 1h30'

Speaker: [Alberto Carta](#) / [Chiara Cignarella](#) / [Nelson Dzade](#) / [George Manyali](#) / [James Sifuna](#) / [Fatema Mohamed](#) / [Omamuyovwi Rita Jolayem](#) / [Maram Ali Ahmed Musa](#)

20:00 Evening session 1h

Speaker: [Christian Carbogno](#) "*FHI-aims: All-Electron, Full-Potential Electronic-Structure Theory with Numeric Atomic Orbitals*"

Friday, June 13 (Day 5)

09:00 Intro to statistical mechanics and Molecular Dynamics 1h

Speaker: [Sara Bonella](#)

10:00 Coffee Break 30'

10:30 Molecular dynamics 2h

Speaker: [Edrick Gonzales](#)

12:30 Lunch Break 1h30'

14:00 Discussion: Q&A

14:30 Hands-on: Molecular dynamics 1h30'

Speaker: [Edward Donkor](#) / [Sara Bonella](#) / [Edrick Solis Gonzalez](#) / [Delchere Don-Tsa](#)

16:00 Coffee Break 30'

16:30 Hands-on: Molecular dynamics 1h30'

Speaker: [Edward Donkor](#) / [Sara Bonella](#) / [Edrick Solis Gonzalez](#)

WEEK 1: ADVANCED SESSION

Monday, June 9 (Day 1)

08:00 Together with the Basic group 6h

14:00 Why should I study more than Kohn-Sham DFT? 2h

Speaker: [Matteo Gatti](#) + [Fatema Mohamed](#) + [Iurii Timrov](#) + [Michele Pavanello](#)

16:00 - onwards Together with the Basic group

Tuesday, June 10 (Day 2)

08:30 Together with the Basic group 1h30'

10:00 Coffee Break 30'

10:30 Advanced xc functionals (DFT+U, hybrids, meta-GGA, and van der Waals) 2h

Speaker: [Iurii Timrov](#)

12:30 Lunch Break 1h30'

14:00 Discussion: Q&A

14:30 Hands-on: Advanced xc functionals (DFT+U and hybrids) 1h30'

Speaker: [Iurii Timrov](#) / [Alberto Carta](#) / [Garu Gebreyesus](#)

16:00 Coffee Break 30'

16:30 Hands-on: Advanced xc functionals (meta-GGA and van der Waals) 1h30'

Speaker: [Iurii Timrov](#) / [Alberto Carta](#) / [Garu Gebreyesus](#)

Wednesday, June 11 (Day 3)

09:00 TDDFT for solids 2h

Speaker: [Matteo Gatti](#) + [Fatema Mohamed](#) + [Iurii Timrov](#)

11:00 Coffee Break 30'

11:30 Orbital-free TDDFT 1h

Speaker: [Michele Pavanello](#)

12:30 Lunch Break 1h30'

14:00 Discussion: Q&A

14:30 Hands-on: TDDFT for solids (for plasmonics) using Quantum ESPRESSO 1h30'

Speaker: [Iurii Timrov](#)

16:00 Coffee Break 30'

16:30 Hands-on: Orbital-free TDDFT (for plasmonics) using DFTpy 1h30'

Speaker: [Michele Pavanello](#)

Thursday, June 12 (Day 4)

09:00 Time-dependent density-functional theory (TDDFT) for molecules 1h30'

Speaker: [Mark Casida](#)

10:30 Coffee Break 30'

11:00 Hands-on: TDDFT for molecular systems using deMon 1h30'

Speaker: [Mark Casida](#)

12:30 Lunch Break 1h30'

14:00 Discussion: Q&A

14:30 Advanced Phonon Lecture & Hands-On: Anharmonicity, Phonon-Phonon, and Electron-Phonon Coupling (*FHI-aims*) 1h30'

Speaker: [Christian Carbogno](#) / [Christoph Dähn](#)

16:00 Coffee Break 30'

16:30 Advanced Phonon Lecture & Hands-On: Anharmonicity, Phonon-Phonon, and Electron-Phonon Coupling (*FHI-aims*) 1h30'

Speaker: [Christian Carbogno](#) / [Christoph Dähn](#)

Friday, June 13 (Day 5)

09:00 Introduction to statistical mechanics and Molecular Dynamics 1h

Speaker: [Sara Bonella](#)

10:00 Coffee Break 30'

10:30 Advanced molecular dynamics: Rare events 2h

Speaker: [Sara Bonella](#)

12:30 Lunch Break 1h30'

14:00 Discussion: Q&A

14:30 Hands-on: Advanced molecular dynamics 1h30'

Speaker: [Sara Bonella](#) / [Edward Donkor](#)

16:00 Coffee Break 30'

16:30 Hands-on: Advanced molecular dynamics 1h30'

Speaker: [Sara Bonella](#) / [Edward Donkor](#)

WEEK 2 : BASIC + ADVANCED SESSION

Monday

09:00 Machine learning 2h

Speakers: [Edward Donkor](#) (1.5 hrs) + [Houlong Zhuang](#) (0.5 hrs)

11:00 Coffee Break 30'

11:30 Machine learning (continuation) 1h

Speakers: [Edward Donkor](#) + [Houlong Zhuang](#)

12:30 Lunch Break 1h30'

14:00 Hands-on: Machine learning 4h

Speakers: [Edward Donkor](#) (1.5-2 hrs) + [Houlong Zhuang](#) (1.5-2 hrs)

Tuesday

09:00 Introduction to quantum computing for ASESMA participants 2h

Speaker:

11:00 Coffee Break 30'

11:30 Project presentations 1h

12:30 Lunch Break 1h30'

14:00 Project presentations 1h

15:00 Public lectures on quantum computing 2h30'

17:30 Round table: the future of quantum

Wednesday

09:00 Special topic lecture 1h (Correlated materials)

Speaker: [Richard Martin](#)

10:00 Special topic lecture 1h (Dynamical mean field theory / strongly correlated materials)

Speaker: [Alberto Carta](#)

11:00 Coffee Break 30'

11:30 Special topic seminar 1h (Electronic structure calculations for energy materials)

Speaker: [Piotr Kowalski](#)

12:30 Lunch break 1h30'

14:00 Special topic seminar 1h (SIESTA)

Speaker: [Javier Junquera](#)

15:00 Projects 3h30'

Thu and Fri: Projects