

**SCHOOL REPORT**  
**ETHIOPIAN SCHOOL ON ELECTRONIC STRUCTURE METHODS AND**  
**APPLICATIONS FOR EMERGING ENERGY TECHNOLOGIES**

Addis Ababa University, College of Natural & Computational Sciences, Addis Ababa, Ethiopia

November 24-December 2, 2021

The lectures and hands-on sessions were delivered by

<b>S/No</b>	<b>Name of Speaker</b>	<b>Institute</b>
1	Dr. Omololu Akin-Ojo	ICTP-IAER, Rwanda
2	Dr. Kingsley Obodo	North-West University, South Africa
3	Dr. Anne Etindele	University of Yaounde, Cameroon
4	Dr. Iurii Timrov	Marvel-EFFL, Switzerland
5	Dr. Getachew Gizaw	Addis Ababa University, Ethiopia
6	Dr. Yedilfana Setarge	Addis Ababa University, Ethiopia
7	Dr. Tamiru Teshome	Addis Ababa Science & Technology University, Ethiopia
8	Mesfin Diro	Addis Ababa University, Ethiopia
9	Dr. Gamachis Sakata	Metu University, Ethiopia
10	Dr. Natei Ermias	Addis Ababa University, Ethiopia
11	Dr. Addisu Gizahegn	Addis Ababa University, Ethiopia
12	Dr. Wondimagegnehu Beshah	Robee Teachers' College, Ethiopia
13	Dr. Genene Shiferaw	Debre Birhan University, Ethiopia
14	Frew Gashaw	Addis Ababa University, Ethiopia

## WEEK-I

24-Nov Wednesday	25-Nov Thursday	26-Nov Friday	27-Nov Saturday	28-Nov Sunday
<b>Morning -Session 9:00 -12:30</b>				
<b>9:00 – 10:10:</b> From Hamiltonian to DFT (session1) (Omololu)	From Hamiltonian to DFT (session2) Omololu,	From Hamiltonian to DFT (session3)	Introduction to classical MD (force field) Getachew	
Break 10:10 – 10:30				
<b>10:30 – 11 :30</b> xc functionals and pseudopotentials (Kingsley)	Crystals, Bloch Theory. Structure relaxation, Band structure. Dr. Kingsley	Phonons (theory) Dr. Anne Dr. Getachew	<i>Ab initio</i> MD Getachew and Tamiru	
<b>11:30 – 12 :30</b>				
Linux, hpc commands, Kingsley, Anne, and Mesfin	Kpoint and lattice parameter (hand-on) Kingsley and Genene	Phonon (hand-on) Phonon DOS & Band St. Anne and Getachew	Classical MD (hand-on) Getachew and Frew	
Lunch – 12:30 – 13:30				
<b>Afternoon – 13:30 – 17:30</b>				
Xcrysden, Xmgrace, Jmol, vesta, Introduction to QE (hand-on Ecut) Anne, Kingsley and Gamachis	vc-relaxation, DOS, PDOS, and BANDS Kingsley and Wondimagegn	>>	<i>Ab initio</i> MD Tamiru and Gamachis	>>

## WEEK-II

WEEK 2- 29-Nov Monday	30-Nov Tuesday	1-Dec Wednesday	2-Dec Thursday
<b>Morning- Session: 8:30 – 10:15</b>			
GPAW Introduction Yedilfana and Natei	GPAW tutorials (DOS, PDOS, and Band structure) Gamachis Asnake Natei, Yedilfana	Advanced functionals (DFT+U and DFT+U+V) Iurii	Machine Learning (ML) for materials science applications Mesfin and Addisu
<b>Break – 10:15 – 10:45.</b>			
<b>Morning – Session 2, 10:45 – 12:30</b>			
GPAW tutorials (optimization hands- on) Gamachis and Asnake	GPAW tutorial	DFT+U and DFT+U+V tutorials and hands-on Iurii, Kingsley and Anne	ML Tutorial Mesfin, Addisu and Gamachis
<b>Lunch: 12:30 – 13:30</b>			
<b>Afternoon: 13:30 – 17:30</b>			
GPAW tutorial continue	GPAW tutorial	DFT+U and DFT+U+V continue	Closing remarks and certification

## List of Participants

<b>S/no</b>	<b>Full Name</b>	<b>Organization</b>
2	Jenbrie Molla	Addis Ababa University
3	Gebrehiwot Gebreslassie	AASTU
4	Gabriel Gashahun	Addis Ababa University
5	Mulugeta Shiferaw	Jimma University
6	Mulugetta Duressa	Jimma University
7	Frew Gashaw	Addis Ababa University
8	Abraham Molla Wagaye	AASTU
9	Adem Siraj	AASTU
10	Belete Sirahbizu	AASTU
11	Aseres Alula	Addis Ababa University
12	Desalegn Nigatu	Addis Ababa University
13	Misganaw Tsegaye	Addis Ababa University
14	Mehbuba Ahmed	ESSTI, AAU
15	Demelie Yimer	Addis Ababa University
16	Alebel Nibret	Bahir Dar University
17	Abebe Tadesse Mulatu	Mekelle University
18	Tsigie Getie Adane	University of Gondar
19	Tamiru Teshome	AASTU
20	Menberu Mengesha	Jimma University
21	Jemal Mohammed	Addis Ababa University
22	Birhan Tesfaye	Mekelle University
23	Natei Ermias Benti	Wolaita Sodo University
24	Tamirat Yibka	Wolaita Sodo University
25	Mengistu Gemech	Bahir Dar University
26	Maru Dessie	Bahir Dar University
27	Eninges Asmare	Wollo University
28	Wondimagegnehu Beshah	AAU
29	Anley Gesese Tesfaye	Jigjiga University
30	Asnake Sahele Haile	Addis Ababa University
31	Tsegaye Bojago Dado	Wolaita Sodo University
32	Solomon Gunta Gutulo	Wolaita Sodo University
33	Getachew Denbela Loko	Addis Ababa University
34	Mesfin Asfaw	ASTU
35	Kunsa Hahu	ASTU
36	Shiferaw Gadisa	Wachemo University
37	Seyfen Kelil	Jigjiga University
38	Georgies Alene	AAiT

39	Teshome Gerbaba Edossa	Wolega University
40	Lemessa Asefa Eressa	Ambo University
41	Menbere Woldetsadik	ASTU
42	Yilak Alemu	Wollega University
43	Tsegaye Belege Atisme	AASTU
44	Alemayehu Dubale	EBti
45	Liya Gebrehiwot	Hawassa
46	Genene Shiferaw	AAU
47	Gamachis Sakata Gurmesa	AAU
48	Zelege Deressa Gerbi	Ambo University
49	Amaregn Kassaye wabeto	Wachemo University
50	Teshome Abute Lelisho	Hawassa University
51	Girma Mekonnen Gomoro	Assosa University
52	Tesfaye Mamo	AAU
53	Eshetu Leka Burayu	Metu University
54	Abire Huluka Fuli	Metu University
55	Gemechu Feyisu Yadeta	Metu University
56	Milkessa Fanta Sima	Metu University
57	Megersa Abdissa Debelo	Metu University
58	Andebet Gedamu	Kotebe MU
59	Hailemariam Teka	Tech and Invo Mins
60	Tsegaye Atisme	Addis Ababa University
61	Yigermal Yassabie	WKU
62	Abel Assefa	Addis Ababa University
63	Girum Adera	AASTU
64	Tesfahun Lejubo	Hawassa University
65	Teshome Lelisho	Hawassa University
66	Tewodros Eyob	Addis Ababa University
67	Wubshet Getachew	Woldia University
68	Yenesew Asrada	Injibara University
69	Mesfin Diro	Addis Ababa University

## Organizers

The organizers of this school were:

- Dr. Yedilfana Setarge Mekonnen, Addis Ababa University
- Dr. Ahmed Mustefa, Addis Ababa University
- Dr. Chernet Amente, Addis Ababa University
- Mr. Mesfin Diro, Addis Ababa University
- Dr. Georgies Alene, Addis Ababa University
- Mr. Frew Gashaw, Addis Ababa University

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