| | Day 0(May 30th) Friday | Day 1 (May 31st) Saturday | Day 2 (June 1st) Sunday | | Day 3 (June 2nd) Monday | | Day 4 (June 3rd) Tuesday | | Day 5 (June 4th) Wednesday | Day 6 (June 5th) Thursday | | Day 7 (June 6th) Friday | | Day 0 (June 7th) Saturday |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **08:45** | | Introduction (Directors & IT) | | | | | | | | | | | | |
| **9:00-9:45 AM** | Arrivals | Direct and reciprocal space, structure factor A. EGGEMAN | Basics of Quantum Chemistry (non-periodic) - Orca F. KLEEMISS Gr1. Beginners | SC Xray Data Reduction - APEX C. LENCZYK, L. KRAUSE Gr2. Beginners | XD part 1 P. MACCHI Gr1. Beginner | Tonto part 1 D. JAYATILAKA Gr2. Beginner | MoPro Part 1 C. JELSCH Gr1. Beginner | HAR in Olex2 F. KLEEMISS Gr2. Beginner | Machine learning in crystallography L. WESTERMAYR | Periodic Quantum Chemistry - Crystal part 1 S.M. CASASSA Gr.1 Intermediate | Periodic Quantum Chemistry - Quantum Expresso part 1 J. KLIMES Gr2. Beginner | ELMOs A. GENONI Gr1. Beginner | Thermal motion treatment A. HOSER Gr2. Beginner | Departures |
| **9:45-10:30 AM** | | Diverse approximations for atomic scattering factors P. DOMINIAK | SC Xray Data Reduction - CryslAlisPRO C.SCHURMANN, A. HOSER Gr1. Beginners | Basics of Quantum Chemistry (non-periodic) - Orca F. KLEEMISS Gr2. Intermmediate | XD part 2 P. MACCHI Gr1. Beginner | Tonto part 2 D. JAYATILAKA Gr2. Beginner | MoPro Part 2 C. JELSCH Gr1. Beginner | TAAM in Olex2 P.DOMINIAK Gr2. Beginner | AI in crystallography, AlphaFold M. Tsenkov | Periodic Quantum Chemistry - Crystal part 2 S.M. CASASSA Gr.1 Intermediate | Periodic Quantum Chemistry - Quantum Expresso part 2 J. KLIMES Gr2. Beginner | Thermal motion treatment A. HOSER Gr1. Beginner | ELMOs A. GENONI Gr2. Beginner | |
| **10:30-11:00 AM** | | Coffee break | Coffee break | | Coffee break | Coffee break | Coffee break | Coffee break | Coffee break | Coffee break | Coffee break | Coffee break | Coffee break | |
| **11:00-11:45 AM** | | Accurate X-ray diffraction measurements L. KRAUSE | Olex2 - structure solution and IAM refinement H. PUSCHMANN Gr1. Beginners | SC Xray Data Reduction - CryslAlisPRO C.SCHURMANN, A. HOSER Gr2. Intermadiate | Tonto part 1 D. JAYATILAKA Gr1. Beginner | XD part 1 P. MACCHI Gr.2 Intermediate | HAR in Olex2 F. KLEEMISS Gr1. Intermediate | MoPro part1 C. JELSCH Gr2. Beginner | Prospects of time resolved crystallography A. MEENTS | Periodic Quantum Chemistry - Quantum Expresso part 1 J. KLIMES Gr.1 Intermediate | Periodic Quantum Chemistry - Crystal part 1 S.M. CASASSA Gr2. Beginner | PolaBer A. KRAWCZUK Gr1. Beginner | XHARPy P.N. RUTH Gr2. Beginner | |
| **11:45-12:30** | | Structure solution and refinement (IAM) H. PUSCHMANN | SC Xray Data Reduction - APEX C. LENCZYK, L. KRAUSE Gr1. | Olex2 - structure solution and IAM refinement H. PUSCHMANN Gr2. Intermediate | Tonto part 2 D. JAYATILAKA Gr1. Beginner | XD part 2 P. MACCHI Gr.2 Intermediate | TAAM in Olex2 P.DOMINIAK Gr1. Beginner | MoPro part2 C. JELSCH Gr2. Beginner | Charge density analysis in 3D ED L. PALATINUS | Periodic Quantum Chemistry - Quantum Expresso part 2 J. KLIMES Gr.1 Intermediat | Periodic Quantum Chemistry - Crystal part 2 S.M. CASASSA Gr2. Beginner | XHARPy P.N. RUTH Gr1. Beginner | PolaBer A. KRAWCZUK Gr2. Beginner | |
| **12:30-2:30 PM** | | Lunch | Lunch | | Lunch | | Lunch | | Lunch | Lunch | | Lunch | | |
| **2.30-3.15 PM** | | Basic Crystallography | Multipole model P.DOMINIAK | | Periodic Quantum Chemistry S.M. CASASSA | | Topological analysis J. CONTRERAS | | Excursion | One-electron reduced density matrix reconstruction J.M. GILLET | | Quantum crystallography in inorganic and bio- organic chemistry S. GRABOWSKY | | |
| **3.15-4:00 PM** | | Basics of Quantum Chemistry A. M. PENDAS | Multipolar electron density data banks C. JELSCH | | ELMOs in Quantum Crystallography A. GENONI | | Topological analysis - Critic2 J. CONTRERAS | | | Dipolar polarizability and applications A. KRAWCZUK | | Quantum refinement for biological applications U. RYDE | | |
| **4:00-4.30 PM** | | Coffee break | Coffee break | | Coffee break | | Coffee break | | | Coffee break | | Coffee break | | |
| **4:30-5.15 PM** | | Dynamics of crystals, introduction to diffuse scattering. A.O. MADSEN | Hirshfeld Atom Refinement (HAR) S. GRABOWSKY | | Introduction to neutron diffraction, Laue experiment A. EDWARDS | | Bonding analyses A. M. PENDAS | | | Bonding analyses - AIMAll A. M. PENDAS | | Women in Crystallography - Round Table, A. KRAWCZUK San Domenico | | |
| **5:15-6:00 PM** | | Crystal structure prediction S. PRICE | X-ray Constrained Wavefunction fitting D. JAYATILAKA | | Neutron diffraction and spin resolved electron density N. CLAISER | | Bonding analyses A. M. PENDAS | | | Bonding analyses - AIMall A. M. PENDAS | | The historical background and future prospects of quantum crystallography P. MACCHI | | |
| **6:00 -6.20 PM** | | Introduction to Erice M.U. SCHMIDT | Poster session Odd numbers | | Quantum Crystallography in materials science B. B. IVERSEN (45 minutes) | | Poster session Even numbers | | | | | Closing for both schools (30 minutes) | | |
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| **8:00 PM-...** | Get together party | Welcome buffet | Dinner at posters | | | | Dinner at posters | | | | | Farewell dinner | | |