

| Hour | Monday 25 | Tuesday 26 | Wednesday 27 | Thursday 28 | Friday 29 |
|---------------|--|--|--|---|---|
| 10:00 - 11:30 | | Atmol Course C. Bunge IF - UNAM | Course On Software For Ab-Initio Calculations H. Rivera Fac. Quimica - UNAM | Course On Software For Ab-Initio Calculations H. Rivera Fac. Quimica - UNAM | Artaios course Y. Ortiz IF - UNAM |
| 11:30 - 12:00 | Cofee Break | Cofee Break | Cofee Break | Cofee Break | Cofee Break |
| 12:00 - 13:00 | Atmol Course C. Bunge IF - UNAM | Alejandro Trejo "First principles study of the vibrational properties of semiconductor nanostructures" IPN | Atmol Course C. Bunge IF - UNAM | "Estabilidad del anión de la molécula de Metano" Guillermo Hinojosa - UNAM Alejandro Ramirez - UAEM | Saul Herrera "Kubo conductivity for anisotropic tilted Dirac semimetals and its application to 8-Pmmn borophene: Role of frequency, temperature, and scattering limits" IF - UNAM |
| 13:00 - 13:30 | | José Santana "Estudio de las nanoestructuras de silicio para su posible aplicación en sensores" IPN | | Juan Chavez "Propiedades electronicas de nanoalambres de silicio para aplicaciones en baterías recargables usando modelos teóricos" | Israel Gonzalez "Estudio de las propiedades físicas de nanoestructuras semiconductoras de silicio aplicadas a dispositivos de almacenamiento de energía" |
| 13:30 - 15:00 | Lunch Break | Lunch Break | Lunch Break | Lunch Break | Lunch Break |
| 15:00 - 16:00 | DFT course Y. Ortiz IF - UNAM | Jorge Martín del Campo "Asymmetric density fitting with modified Cholesky decomposition applied to second order electron propagator" Fac. Quimica - UNAM | DFT course Y. Ortiz IF - UNAM | DFT course Y. Ortiz IF - UNAM | Jose Eduardo Gonzalez "Thermoelectric transport in poly(G)-poly(C) double chains" IPN |
| 16:00 - 16:30 | | Cofee Break | | | |
| 16:30 - 17:00 | Cofee Break | | Cofee Break | Cofee Break | |
| 17:00 - 17:30 | Thomas Stegmann "Quantum Transport" ICF - UNAM | Course On Software For Ab-Initio Calculations H. Rivera Fac. Quimica - UNAM | Alma Marcos "Efecto de la dimensionalidad en las propiedades electrónicas de semiconductores binarios" IPN | Hector Muñoz "Propiedades electrónicas y de adsorción del carburo de germanio bidimensional aplicado al almacenamiento de hidrógeno" | |
| 17:30 - 18:00 | | | | | |

| Hour | Monday 18 | Tuesday 19 | Wednesday 20 | Thursday 21 | |
|-------|---|--|--|--|--|
| 9:30 | | | | | |
| 10:00 | <p>Carlos Bunge "Brief Exposition of the Correlation Problem" IF-UNAM</p> | <p>Thom Dunning "Casting Aside Delimitations of Molecular Orbital Theory" University of Washington</p> | <p>Thom Dunning "Quantitative Quantum Chemistry" University of Washington</p> | <p>Robert Morrison "Temporary Anion States: Future Work and Problems to be Solved" East Carolina University</p> | |
| 10:30 | | | | | |
| 11:00 | | Coffee Break | | | |
| 11:30 | Coffee Break | <p>Alberto Vela "Robust Prediction of Spin Crossover in Transi- tion Metal Complexes. Are DFT approximations capable of describing this problem" CINVESTAV</p> | Coffee Break | | |
| 12:00 | <p>Robert Morrison "Temporary Anion Resonance States, non-Hermitian Quantum Mechanics, Chemical Reactivity, Uncertainty and the Pauli Principle" East Carolina University</p> | | <p>Ignacio Garzón "Quiral Nanostructures: A DFT Approach" IF-UNAM</p> | <p>Humberto Saint-Martin Posada "Theoretical Studies of the Hydration of Small Molecules. From the Gas Phase to the Aqueous Solution" ICF - UNAM</p> | |
| 12:30 | | <p>Jorge Garza "Use of Graphics Processing Units in Quantum Chemistry" UAM-I</p> | | | |
| 13:00 | | | | | |
| 13:30 | | | | | |
| 14:00 | Lunch Break | Lunch Break | Lunch Break | Lunch Break | |
| 14:30 | | | | | |
| 15:00 | <p>Álvaro Vázquez-Mayagoitia "Dynamic Polarizabilities Calcula- ted with Time-Dependent ab initio Methods with Multiresolution Multiwavelet Basis Sets" Argonne National Laboratory</p> | <p>Álvaro Vázquez-Mayagoitia "Auto-Generated Data Sets for Engineering co-Sensitized Solar Cells and its Applications" Argonne National Laboratory</p> | <p>Andreas Köster "Auxiliary Density Functional Theory: A Bridge between DFT and ab-initio Methods?" CINVESTAV</p> | <p>Omar de la Peña Seaman "Superconductivity in Metallic Hydrides: How Important is to put them Under Pressure" IF - BUAP</p> | |
| 15:30 | | | | | |
| 16:00 | | | | | |
| 16:30 | Coffee Break | | | | |
| 17:00 | <p>Carlos Jimenez-Hoyos "Quantum Chemistry Using non-Orthogonal Determinant Expansions" Wesleyan University</p> | <p>Audience Under Moderator "Present and Future of ab initio work"</p> | <p>Patrizia Calaminici "IR and Raman Spectra of Nanosystems from Auxiliary Density Functional" CINVESTAV</p> | | |
| 17:30 | | | | | |
| 18:00 | | | | | |
| 18:30 | | | | | |