“Bridging the gap between theory and experiment: which theoretical approaches are best suited to solve real problems in nanotechnology and biology?”

Stanford University, February 23-26

Workshop Program

**Location:** 101X Auditorium, Paul G. Allen Building

**Tuesday, February 23**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Chair/Presenter</th>
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<tbody>
<tr>
<td>7.30-8.00 am</td>
<td>Continental Breakfast</td>
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<tr>
<td>8.00-8.05 am</td>
<td>Opening Remarks</td>
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<tr>
<td>8.05-8.45 am</td>
<td><strong>Steven Louie</strong> Physics of Graphene and Graphene Nanostructures</td>
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<tr>
<td>8.45-9.25 am</td>
<td><strong>Alex Demkov</strong> First Principles Theory and Materials R&amp;D</td>
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<tr>
<td>9.25-10.05 am</td>
<td><strong>Gennadi Bersuker</strong> Identifying Structure-Performance Relations in the Advanced Gate Stacks</td>
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<tr>
<td>10.05-10.20 am</td>
<td>Coffee Break</td>
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<tr>
<td>10.20-11.00 am</td>
<td><strong>Jim Chambers</strong> Metal Gate Electrode Impurity Engineering for Control of Effective Work Function</td>
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<td>11.00-11.40 am</td>
<td><strong>Anderson Janotti</strong> Defects and Impurities in Oxide Semiconductors: What Have We Learned so Far?</td>
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<tr>
<td>12.00-1.00 pm</td>
<td>Lunch</td>
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**Chair: Gennadi Bersuker**

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<tbody>
<tr>
<td>1.00-1.40 pm</td>
<td><strong>Giulia Galli</strong> Integrate Theory, Computation and Experiment: the Role of Quantum Simulations</td>
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<tr>
<td>1.40-2.20 pm</td>
<td><strong>Kyeongjae Cho</strong> Multiscale Design of Catalyst Nanoparticles: from Concepts to Commercial Applications</td>
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<tr>
<td>2.20-3.00 pm</td>
<td><strong>Shela Aboud</strong> Density Functional Theory Studies of Oxides and Nanoparticles</td>
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<tr>
<td>3.00-3.15 pm</td>
<td>Coffee Break</td>
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**Chair: Alex Demkov**

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<tbody>
<tr>
<td>3.15-3.55 pm</td>
<td><strong>Vijay Pande</strong> Folding@home: New Algorithms and Computational Paradigms for Simulating Biological Systems in Atomic Detail on the Millisecond Timescale</td>
<td></td>
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<tr>
<td>3.55-4.35 pm</td>
<td><strong>Erik Lindahl</strong> Modeling Membrane Proteins with Computers</td>
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<tr>
<td>4.35-5.15 pm</td>
<td><strong>Olav Solgaard</strong> Nanoscale Material Characterization with Differential Interferometric Atomic Force Microscopy</td>
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<tr>
<td>Time</td>
<td>Session</td>
<td>Speakers</td>
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<tr>
<td>8.00-8.40 am</td>
<td>Nanophotonic Devices for Classical and Quantum Information Processing</td>
<td>Yiyang Gong, Jelena Vuckovic</td>
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<tr>
<td>8.40-9.20 am</td>
<td>Nanophotonics Theory and Simulations</td>
<td>Zongfu Yu, Shanhui Fan</td>
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<tr>
<td>9.20-10.00 am</td>
<td>Are Quasiparticles Resolvable in Measurements of Threshold Voltage and Mobility at Finite Temperatures?</td>
<td>Brendan McDougall</td>
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<tr>
<td>10.00-10.15 am</td>
<td>Coffee Break</td>
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<tr>
<td>10.15-10.55 am</td>
<td>Atomistic Simulations of Nanoelectronic Devices</td>
<td>Mathieu Luisier</td>
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<td>10.55-11.35 am</td>
<td>Hybrid Methods for Device Simulations</td>
<td>Simon Brugger</td>
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<td>11.35-12.15 pm</td>
<td>Quantum Transport Simulation: A few Case Studies Where It is Necessary</td>
<td>Sayeef Salahuddin</td>
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<tr>
<td>12.30-1.30 pm</td>
<td>Lunch</td>
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<tr>
<td>1.30-2.10 pm</td>
<td>Leveraging Simulations to Gain Insights into Polymer Electrolyte Fuel Cells</td>
<td>Lalitha Subramanian</td>
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<tr>
<td>2.10-2.50 pm</td>
<td>Bridging the Gap between Novice Users and High Quality Microsecond Scale Simulations in the Biological Sciences Using Desmond</td>
<td>Istvan Kolossvary</td>
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<tr>
<td>2.50-3.05 pm</td>
<td>Coffee Break</td>
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<tr>
<td>3.05-3.45 pm</td>
<td>Advanced Optimization and Sampling Algorithms in Structure Based Biocomputing: From Chain Closure to Variable Transformations</td>
<td>Péter Mináry</td>
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<tr>
<td>3.45-4.25 pm</td>
<td>Computational Needs for the Study of Implantable Medical Devices</td>
<td>Ada Poon</td>
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<tr>
<td>4.25-5.05 pm</td>
<td>Large Scale Models in Neuroscience: Simulating the Activity of the Visual Cortex</td>
<td>Călin Buia</td>
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### Thursday, February 25th

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<tr>
<td>7.30-8.00 am</td>
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<tr>
<td>8.00-9.00 am</td>
<td><strong>Anders Blom</strong>&lt;br&gt;Theoretical Methodologies Implemented in ATK, VNL and SE (QuantumWise)</td>
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<tr>
<td>9.00-10.00 am</td>
<td>ATK Tutorial - Part I</td>
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<tr>
<td>10.00-10.15 am</td>
<td>Coffee Break</td>
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<tr>
<td>10.15-11.15 am</td>
<td>ATK - User Presentations</td>
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<tr>
<td>11.15-12.00 pm</td>
<td>ATK Tutorial - Part II</td>
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<tr>
<td>12.00-1.00 pm</td>
<td>Lunch</td>
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<tr>
<td>1.00-2.45 pm</td>
<td>Hands-on Training ATK/VNL/SE - Part I</td>
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<td>2.45-3.00 pm</td>
<td>Coffee Break</td>
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<tr>
<td>3.00-3.30 pm</td>
<td><strong>Christopher Bruns</strong>&lt;br&gt;Introduction to OpenMM for accelerating molecular dynamics on GPUs (SIMBIOS)</td>
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<tr>
<td>3.30-5.00 pm</td>
<td>Hands-on tutorial with OpenMM Zephyr (SIMBIOS)</td>
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### Friday, February 26th

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<tr>
<td>7.30-8.00 am</td>
<td>Continental Breakfast</td>
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<tr>
<td>8.00-9.00 am</td>
<td><strong>Anders Blom</strong>&lt;br&gt;ATK - Q&amp;A, Follow-up from Tutorial Sessions</td>
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<tr>
<td>9.00-10.00 am</td>
<td>Hands-on Training ATK/VNL/SE - Part II</td>
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<tr>
<td>10.00-10.15 am</td>
<td>Coffee Break</td>
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<tr>
<td>10.15-12.00 pm</td>
<td>ATK/VNL/SE Discussions on Future Development Plans, Features, etc.</td>
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<td>12.00-1.00 pm</td>
<td>Lunch</td>
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<tr>
<td>1.00-2.45 pm</td>
<td><strong>István Kolossváry</strong>&lt;br&gt;Desmond Tutorial (DE Shaw Research)</td>
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<td>2.45-3.00 pm</td>
<td>Coffee Break</td>
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<tr>
<td>3.00-5.00 pm</td>
<td>Desmond Hands-on Training (DE Shaw Research)</td>
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