

## Efthimios Kaxiras

### I. CURRICULUM VITAE

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**Education:** *Massachusetts Institute of Technology*

Ph.D. in Physics	1987
B.S. in Physics	1981
<i>National Technical University of Athens, Greece</i>	1977-78
Electrical Engineering (transferred to MIT)	

**Positions:** *Gordon McKay Professor of Applied Physics and Professor of Physics* 1998-  
*Associate Professor of Physics and Applied Physics* 1995-98  
*Assistant Professor of Physics and Applied Physics* 1991-95  
Department of Physics and School of Engineering and Applied Sciences  
Harvard University  
*Associate Director* 2001-02  
Materials Research Science and Engineering Center, Harvard University  
*Director* 2002-04  
Biomedical Research Institute, Foundation for Research and Technology - Hellas  
*Visiting Professor and Acting Chair* 2002-04  
Department of Materials Science and Technology, University of Ioannina - Greece  
*Affiliated Scientist* 1996-  
Institute of Electronic Structure and Lasers, FORTH – Greece  
*Consulting Research Physicist* 1989-91  
Complex Systems Theory Branch, Naval Research Laboratory, Washington  
*Postdoctoral Research Associate* 1987-89  
IBM Research Division, T.J. Watson Research Center, Yorktown Heights

**Honors:**

- IBM Research Division Award (1991)  
“*For contributions to the development of a new mechanism for Si/Ge heteroepitaxy*”
- IBM Predoctoral Fellowship (1985-87)
- Chartered Physicist and Fellow of the Institute of Physics (London), since 1999
- Fellow of the American Physical Society, since 2003

**Professional Activities:**

- Member of: American Physical Society, Materials Research Society, American Chemical Society, Sigma Xi - Scientific Research Society, Institute of Physics.
- Editorial Board of
  - *Modelling and Simulation in Materials Science and Engineering*
  - *Journal of Computer Aided Materials Design*
  - *Surface Review and Letters*
  - *International Journal for Multiscale Computational Engineering*
  - *Computing in Science and Engineering* (Advisory Committee)

### **Organization of Scientific Meetings:**

- Co-organizer of Conference on “*Synergy Between Experiment and Computation in Nanoscale Science*”, National Nanoscale Infrastructure Network, Harvard University (May 2006).
- Co-organizer of Focus Session “*Steps, Growth and Smoothing*”, American Physical Society March Meeting, Baltimore (March 2006).
- Session Organizer: “*Multiscale Simulations in Materials Science*”, SIMU- European Physical Society Workshop on Bridging the Scales, Genova, Italy (August 2004).
- Co-organizer of Workshop on “*Multiscale Modeling and Simulation*”, sponsored by ETH-Z Computational Laboratory, Lugano, Switzerland (August 2003).
- Co-organizer of Workshop on “*Multiscale Modeling of Materials: Methods, Algorithms and Unsolved Problems*”, sponsored by Centre Europeen pour le Calcul Atomique et Moleculaire (CECAM), Heraklion, Greece (July 2001).
- Co-organizer of Symposium on “*New Advances in Materials Prediction*”, Fall 1999 Meeting of the Materials Research Society, Boston.
- Co-organizer of Symposium on “*Multiscale Modeling of Materials*”, Fall 1998 Meeting of the Materials Research Society, Boston.
- Co-organizer of Workshop on “*Multiscale Modeling and Grand Challenge Problems in Materials Research*”, CECAM, Lyon, France (October 1997).
- Co-organizer of Workshop on “*Quantitative Methods in Materials Research*”, Institute of Theoretical Physics, U.C. Santa Barbara (January - June 1997).
- Co-organizer of Symposium on “*Epitaxial Growth: Principles and Applications*”, Spring 1997 Meeting of the Materials Research Society, San Francisco.
- Co-organizer of Symposium on “*Materials Theory, Simulations and Parallel Algorithms*”, Fall 1995 Meeting of the Materials Research Society, Boston.

## **II. PUBLICATIONS**

### **II.1 Books, Invited Reviews and Book Chapters:**

10. “Overview of Multiscale Simulations of Materials”, Gang Lu and E.Kaxiras, *Handbook of Theoretical and Computational Nanotechnology*, Vol. X, pp. 1-33, edited by M. Rieth and W. Schommers (American Scientific Publishers, 2005).
9. “Introduction: Atomistic Nature of Materials”, E. Kaxiras and S. Yip, *Handbook of Materials Modeling*, edited by S. Yip, pp. 451-458, (Springer, Netherlands, 2005).
8. *Atomic and Electronic Structure of Solids*, E. Kaxiras (Cambridge University Press, Cambridge, 2003).
7. *Materials Science*, E. Kaxiras, Guest Editor for collection of articles in *Computing in Science and Engineering*, vol. 3(6) (Nov.-Dec. 2001).
6. “The surfactant effect in semiconductor thin film growth”, D. Kandel and E. Kaxiras, *Solid State Physics*, edited by H. Ehrenreich and F. Spaepen vol. 54, pp.219-262, (Academic Press, San Diego, 2000).

5. *Multiscale Modeling of Materials*, Materials Research Society Symposium Proceedings, vol. 538, edited by V. Bulatov, T. Diaz de la Rubia, R. Phillips, E. Kaxiras and N. Gonhiem (MRS, Pittsburgh, 1999).
4. “Modeling and simulation of solids”, E. Kaxiras and S. Yip, collection of articles edited in *Current Opinion in Solid State and Materials Science*, vol. 3 (1998).
3. “Simulation of Semiconductor Growth Mechanisms in the Presence of Adsorbate Layers”, in *Computational Materials Science*, edited by C.Y. Fong (World Scientific, Singapore, 1997).
2. “Structure and properties of covalently bonded Si clusters”, in *Cluster Assembled Materials*, edited by K. Sattler, Materials Science Forum vol. 232, pp.67-86 (1996).
1. *Materials Theory, Simulations and Parallel Algorithms*, Materials Research Society Symposium Proceedings, vol. 408, edited by E. Kaxiras, J.D. Joannopoulos, P. Vashishta, and R.K. Kalia (MRS, Pittsburgh, 1996).

## II.2 Articles in Refereed Scientific Journals:

177. “Structure of incommensurate gold sulfide monolayer on Au(111)”, S.Y. Quek, M. M. Biener, J. Biener, J. Bhattacharjee, C. M. Friend, U. V. Waghmare, and E. Kaxiras, *J. Chem. Phys. - to appear* (2007).
176. “Multiscale model of electronic behavior and localization in stretched dry DNA”, R.L. Barnett, P. Maragakis, A. Turner, M. Fyta and E. Kaxiras, *J. Mater. Sci.* **42**, 8894-8903 (2007).
175. “Semiconducting cyanide-transition-metal nanotubes”, Y. Mo and E. Kaxiras, *Small* **3**, 1253-1258 (2007).
174. “Diamond stabilization of ice multilayers at human body temperature”, A. Wissner-Gross and E. Kaxiras, *Phys. Rev. E* **76**, 020501(R) (2007).
173. “Exploring DNA translocation through a nanopore via a multiscale lattice-Boltzmann molecular-dynamics methodology”, S. Melchionna, M. Fyta, E. Kaxiras and S. Succi, *Int. J. of Mod. Phys. C* **18**, 685-692 (2007).
172. “Metal-diboride nanotubes as high-capacity hydrogen storage media”, S. Meng, E. Kaxiras and Z.Y. Zhang, *NanoLett.* **7**, 663-667 (2007).
171. “Negative differential resistance in transport through organic molecules in silicon”, S. Y. Quek, J.B. Neaton, M.S. Hybertsen, E. Kaxiras and S.G. Louie, *Phys. Rev. Lett.* **98**, 066807 (2007).
170. “DNA nucleoside interaction and identification with carbon nanotubes”, S. Meng, P. Maragakis, C. Papaloukas and E. Kaxiras, *NanoLett.* **7**, 45-50 (2007).
169. “Multiscale coupling of molecular dynamics and hydrodynamics: application to DNA translocation through a nanopore”, M. G. Fyta, S. Melchionna, E. Kaxiras, and S. Succi, *Multiscale Model. Simul.* **5**, 1156-1173 (2006).
168. “Schottky barrier formation at a carbon nanotube – metal junction”, W. Zhu and E. Kaxiras, *Appl. Phys. Lett.* **89**, 243107 (2006).
167. “Structural model of eumelanin”, E. Kaxiras, A. Tsolakidis, G. Zonios, and S. Meng, *Phys. Rev. Lett.* **97**, 218102 (2006).
166. “Active role of buried ultrathin oxide layers in adsorption of O<sub>2</sub> on Au films”, S.Y. Quek, C.M. Friend and E. Kaxiras, *Surf. Sci.* **600**, 3388-3393 (2006).

165. “Rich coordination chemistry of Au atoms in gold sulfide monolayer on Au(111)”, S.Y. Quek, M.M. Biener, J. Biener, J. Bhattacharjee, C.M. Friend, U.V. Waghmare and E. Kaxiras, *J. Phys. Chem. B- Lett.* **110**, 15663-15665 (2006).
164. “First-principles studies of the electronic structure of cyclopentene on Si(001): density functional theory and GW”, S.Y. Quek, J.B. Neaton, M.S. Hybertsen, E. Kaxiras and S.G. Louie, *Physica Stat. Solid. B* **243**, 2048-2053 (2006).
163. “Theory of spintronic materials”, J.R. Chelikowsky, E. Kaxiras and R.M. Wentzcovitch, *Physica Stat. Solid. B* **243**, 2133-2150 (2006).
162. “Electronic structure of Pd-covered (10,0) carbon nanotube”, W.G. Zhu and E. Kaxiras, *Physica Stat. Solid. B* **243**, 2164-2169 (2006).
161. “Tuning solid surfaces from hydrophobic to superhydrophilic by submonolayer surface modification”, S. Meng, Z.Y. Zhang and E. Kaxiras, *Phys. Rev. Lett.* **97**, 036107 (2006).
160. “The nature of contact between Pd leads and semiconducting carbon nanotubes”, W.G. Zhu and E. Kaxiras, *NanoLett.* **6**, 1415-1419 (2006).
159. “Formation of monatomic Fe chains on vicinal Cu(111) surfaces: An atomistic view”, J.D. Guo, Y. Mo, E. Kaxiras, Z.Y. Zhang, and H.H. Weitering, *Phys. Rev. B* **73**, 193405 (2006).
158. “Embedded atom method potentials employing a faithful density representation”, P. Mitev, G.A. Evangelakis and E. Kaxiras, *Modelling Simul. Mater. Sci. Eng.* **14**, 721-731 (2006).
157. “From electrons to finite elements: a concurrent multiscale approach for metals” G. Lu, E. Tadmor and E. Kaxiras, *Phys. Rev. B* **73**, 024108 (2006).
156. “Orbital-free density functional theory applied to NaAlH<sub>4</sub>”, T.J. Frankcombe, G.J. Kroes, N.I. Choly and E. Kaxiras, *J. Phys. Chem. B* **109**, 16554-16562 (2005).
155. “Superconducting and charge-density wave instabilities in ultrasmall-radius carbon nanotubes”, R. Barnett, E. Demler and E. Kaxiras, *Solid State Comm.* **135**, 335-339 (2005).
154. “Carbon nanotube interaction with DNA”, G. Lu, P. Maragakis and E.Kaxiras, *NanoLett.* **5**, 897-900 (2005).
153. “Multiscale simulations in simple metals: A density-functional-based methodology”, N. Choly, G. Lu, W. E and E.Kaxiras, *Phys. Rev. B* **71**, 094101 (2005).
152. “Hydrogen embrittlement of aluminum: The crucial role of vacancies”, G. Lu and E. Kaxiras, *Phys. Rev. Lett.* **94** (15) 155501 (2005).
151. “Kinetic pathway for the formation of Fe nanowires on stepped Cu(111) surfaces”, Y. Mo, K. Varga, E. Kaxiras and Z. Zhang, *Phys. Rev. Lett.* **94** (15) 155503 (2005).
150. “A TDDFT study of the optical response of DNA bases, base pairs and their tautomers in the gas phase”, A. Tsolakidis and E. Kaxiras, *J. Phys. Chem. A* **109** (10) 2373-2380 (2005).
149. “Tuning electronic properties of novel metal oxide nanocrystals using interface interactions: MoO<sub>3</sub> monolayers on Au(111)”, S.Y. Quek, M.M. Biener, J. Biener, C.M. Friend and E. Kaxiras, *Surface Sci. Lett.* **577**, L71-L77 (2005).
148. “Electron-phonon interaction in ultrasmall-radius carbon nanotubes”, R. Barnett, E. Demler and E.Kaxiras, *Phys. Rev. B* **71**, 035429 (2005).
147. “Sulfur point defects in crystalline and amorphous silicon”, Y. Mo, M.Z. Bazant and E.Kaxiras, *Phys. Rev. B* **70**, 205210 (2004).

146. “Contrasting growth modes of Mn on Ge(100) and Ge(111) surfaces: Subsurface segregation versus intermixing”, W. Zhu, H.H. Weitering, E.G. Wang, E. Kaxiras, and Z. Zhang, *Phys. Rev. Lett.* **93**, 126102 (2004).
145. “Modeling of the carbon-rich c(4x4) reconstruction on Si(100)”, I.N. Remediakis, C. Guedj, P.C. Kelires, D. Grutzmacher, and E. Kaxiras, *Surface Science* **554** (2-3): 90-102 (2004).
144. “Modeling Zinc in biomolecules with the self consistent charge-density functional tight binding (SCC-DFTB) method: Applications to structural and energetic analysis”, M. Elstner, Q. Cui, P. Muni, E. Kaxiras, Th. Frauenheim, M. Karplus, *J. Comput. Chem.* **24** (5), 565-581 (2003).
143. “Dinitrosyl formation as an intermediate stage of the reduction of NO in the presence of MoO<sub>3</sub>”, I.N. Remediakis, E. Kaxiras, M. Chen and C.M. Friend, *J. Chem. Phys.* **118** (13), 6046-6051 (2003).
142. “Fast method for force computations in electronic structure calculations”, N. Choly and E. Kaxiras, *Phys. Rev. B* **67**, 155101 (2003).
141. “Electronic structure of overstretched DNA”, P. Maragakis, R.L. Barnett, E. Kaxiras, M. Elstner and Th. Frauenheim, *Phys. Rev. B* **66**, 241104 (2002).
140. “Adaptive nudged elastic band approach for transition state calculations”, P. Maragakis, S. Andreev, Y. Brumer, D.R. Reichman, E. Kaxiras, *J. Chem. Phys.* **117**, 4651 (2002).
139. “Electronic structure of solid nitromethane: Effects of high pressure and molecular vacancies”, D. Margetis, E. Kaxiras, M. Elstner, Th. Frauenheim, M. Riad Manaa, *J. Chem. Phys.* **117**, 788 (2002).
138. “Kinetic energy density functionals for non-periodic systems”, N. Choly, E. Kaxiras, *Solid State Comm.* **121**, 281 (2002).
137. “A lattice Boltzmann study of reactive microflows”, A. Gabrielli, S. Succi, E. Kaxiras, *Comp. Phys. Comm.* **147**, 516 (2002).
136. “Lattice Boltzmann simulation of reactive microflows over catalytic surfaces”, S. Succi, G. Smith and E. Kaxiras, *J. Stat. Phys.* **107**, 343 (2002).
135. “Can vacancies lubricate dislocation motion in aluminum?”, G. Lu and E. Kaxiras, *Phys. Rev. Lett.* **89**, 105501 (2002).
134. “Polarization switching in PbTiO<sub>3</sub>: an ab initio finite element simulation”, E.B. Tadmor, U.V. Waghmare, G.S. Smith and E. Kaxiras, *Acta Materialia* **50**, 2989 (2002).
133. “Energetics of hydrogen impurities in aluminum and their effect on mechanical properties”, G. Lu, D. Orlikowski, I. Park, O. Politano and E. Kaxiras, *Phys. Rev. B* **65**, 064102 (2002).
132. “Density-functional theory modeling of bulk magnetism with spin-dependent pseudopotentials”, F. Starost, K. Kim, S.C. Watson, E. Kaxiras and E.A. Carter, *Phys. Rev. B* **64**, 235105 (2001).
131. “Variational finite-difference representation of the kinetic energy operator”, P. Maragakis, J. Soler and E. Kaxiras, *Phys. Rev. B* **64**, 193101 (2001).
130. “Multiscale simulation of silicon nanoindentation”, G.S. Smith, E.B. Tadmor, N. Bernstein and E. Kaxiras, *Acta Materialia* **49**, 4089 (2001).
129. “Applying the lattice Boltzmann equation to multiscale fluid problems”, S. Succi, O. Filippova, G. Smith and E. Kaxiras, *Computing in Science and Engineering* **3**, 26 (2001).

128. “Chemical efficiency of reactive microflows with heterogeneous catalysis: a lattice Boltzmann study”, S. Succi, G. Smith, A. Gabrielli, E. Kaxiras, *Europ. Phys. J.: Appl. Phys.* **16**, 71, (2001).
127. “Quantum mechanics simulation of protein dynamics on long timescale”, H. Liu, M. Elstner, E. Kaxiras, Th. Frauenheim, J. Hermans, and W. Yang, *Proteins: Structure, Function and Genetics* **44**, 484 (2001).
126. “A QM/MM implementation of the self-consistent charge density functional tight binding (SCC-DFTB) method”, Q. Cui, M. Elstner, E. Kaxiras, T. Frauenheim and M. Karplus, *J. Phys. Chem. B* **105**, 569 (2001).
125. “Hydrogen bonding and stacking interactions of nucleic acid base pairs: A density-functional-theory based treatment”, M. Elstner, P. Hobza, T. Frauenheim, S. Suhai and E. Kaxiras, *J. Chem. Phys.* **114**, 5149 (2001).
124. “The chemical nature of surface point defects on MoO<sub>3</sub>(010): Adsorption of hydrogen and methyl”, M. Chen, C.M. Friend and E. Kaxiras, *J. Am. Chem. Soc.* **123**, 2224 (2001).
123. “Dislocation core properties of aluminum: a first-principles study”, G. Lu, N. Kioussis, V.V. Bulatov and E. Kaxiras, *Mat. Sci. and Engin. A* **309**, 142 (2001).
122. “HARES: an efficient method for first-principles electronic structure calculations of complex systems”, U.V. Waghmare, H. Kim, I.J. Park, N. Modine, P. Maragakis and E. Kaxiras, *Computer Phys. Comm.* **137**, 341 (2001).
121. “Hydrogen enhanced local plasticity in Aluminum: an ab-initio study”, G. Lu, Q. Zhang, N. Kioussis and E. Kaxiras, *Phys. Rev. Lett.* 095501 (2001).
120. “Thermodynamics of C incorporation in Si(100)”, I.N. Remediakis, E. Kaxiras and P. Kelires, *Phys. Rev. Lett.* **86**, 4556 (2001).
119. “A self-consistent charge density-functional based tight-binding scheme for large biomolecules”, M. Elstner, Th. Frauenheim, E. Kaxiras, G. Seifert and S. Suhai, *Phys. Stat. Sol. B* **217**, 357 (2000).
118. “Generalized stacking fault energy surface and dislocation properties of aluminum”, G. Lu, N. Kioussis, V.V. Bulatov and E. Kaxiras, *Phys. Rev. B* **62**, 3099 (2000).
117. “The Peierls-Nabarro model revisited”, G. Lu, N. Kioussis, V.V. Bulatov and E. Kaxiras, *Phil. Mag. Lett.* **80**, 675 (2000).
116. “Structure of III-Sb(001) growth surfaces: the role of heterodimers”, W. Barvosa-Carter, A.S. Bracker, J.C. Culberson, B.Z. Nosko, B.V. Shanabrook, L.J. Whitman, H. Kim, N.A. Modine and E. Kaxiras, *Phys. Rev. Lett.* **84**, 4649 (2000).
115. “A density functional theory study of site-specific methyl reaction on MoO<sub>3</sub>(010): The effects of methyl coverage”, M. Chen, C.M. Friend and E. Kaxiras, *J. Chem. Phys.* **112**, 9617 (2000).
114. “Energetic, vibrational and electronic properties of silicon using a nonorthogonal tight-binding model”, N. Bernstein, M.J. Mehl, D.A. Papaconstantopoulos, M.Z. Bazant and E. Kaxiras, *Phys. Rev. B* **62**, 4477 (2000); Correction, *Phys. Rev. B* **65**, 249902 (2002).
113. “Atomistic simulations of solid-phase epitaxial growth in silicon”, N. Bernstein, M. J. Aziz and E. Kaxiras, *Phys. Rev. B* **61**, 6696 (2000).
112. “Modeling brittle and ductile behavior of solids from first-principles calculations”, U. V. Waghmare, E. Kaxiras and M. S. Duesbery, *Phys. Stat. Sol. B* **217**, 545 (2000).
111. “Multiscale simulation of loading and electrical resistance in silicon nanoindentation”, G. S. Smith, E. B. Tadmor and E. Kaxiras, *Phys. Rev. Lett.* **84**, 1260 (2000).

110. "Theory of the (3 x 2) reconstruction of the GaAs(001) surface", N.A. Modine and E. Kaxiras, *Mat. Sci. and Engin. B* **67**, 1 (1999).
109. "Resolving discrepancies between LEED and STM through ab initio calculations: Surface structure and bonding of sulfur on Mo(110)", M. Chen, P.G. Clark, Jr., T. Mueller, C.M. Friend and E. Kaxiras, *Phys. Rev. B* **60**, 11783 (1999).
108. "Electronic and optical properties of Si<sub>1-x</sub>C<sub>x</sub> alloys", G. Theodorou, G. Tsegas, P.C. Kelires and E. Kaxiras, *Phys. Rev. B* **60**, 11494 (1999).
107. "Self-organized growth of Ge quantum dots on Si(001) substrates induced by sub-monolayer C coverages", O. Leifeld, R. Hartman, B. Müller, E. Kaxiras, K. Kern and D. Grützmacher *Nanotechnology* **10**, 122 (1999).
106. "Concurrent coupling of length scales: methodology and application", J.Q. Broughton, N. Bernstein, E. Kaxiras and F.F. Abraham, *Phys. Rev. B* **60**, 2391 (1999).
105. "Metal-coated fullerenes: electronic, geometrical and vibrational properties of C<sub>60</sub>M<sub>62</sub> (M=Ti and V)", M.R. Pederson, D.V. Porezag, D.C. Patton and E. Kaxiras, *Chem. Phys. Lett.* **303**, 373 (1999).
104. "Dimer pairing on the C-alloyed Si(001) surface", O. Leifeld, D. Grützmacher, B. Müller, K. Kern, E. Kaxiras and P. Kelires, *Phys. Rev. Lett.* **82**, 972 (1999).
103. "Linking chemical reactivity, magic numbers, and local electronic properties of clusters", D.R. Alfonso, S.-Y. Wu, C.S. Jayanthi and E. Kaxiras, *Phys. Rev. B* **59**, 7745 (1999).
102. "{331} slip on (013) planes in molybdenum disilicide", U.V. Waghmare, E. Kaxiras, V. Bulatov and M.S. Duesbery, *Phil. Mag. A* **79**, 655 (1999).
101. "Microalloying for ductility in molybdenum disilicide", U.V. Waghmare, V. Bulatov, E. Kaxiras, M.S. Duesbery, *Mat. Sci. and Engin. A* **261**, 147 (1999).
100. "Theory of electronic and optical properties of 3c-SiC", G. Theodorou, G. Tsegas and E. Kaxiras, *J. Appl. Phys.* **85**, 2179 (1999).
99. "Band structure calculations for semiconductors within the generalized density functional theory", I.N. Remediakis and E. Kaxiras, *Phys. Rev. B* **59**, 5536 (1999).
98. "Mixed finite element and atomistic formulation for complex crystals", E. Tadmor, G.S. Smith and E. Kaxiras, *Phys. Rev. B* **59**, 235 (1999).
97. "Spanning the continuum to quantum length scales in a dynamic simulation of brittle fracture", F.F. Abraham, J.Q. Broughton, N. Bernstein and E. Kaxiras, *Europhys. Lett.* **44**, 783 (1998).
96. "Atomistic features of the amorphous-crystal interface in silicon", N. Bernstein, M.J. Aziz and E. Kaxiras, *J. of Computer Aided Materials Design* **5**, 55 (1998).
95. "First-principles study of static nano-scale friction between MoO<sub>3</sub> and MoS<sub>2</sub>", G.S. Smith, N.A. Modine, U.V. Waghmare and E. Kaxiras, *J. of Computer Aided Materials Design* **5**, 61 (1998).
94. "Spanning the length scales in dynamic simulation", F.F. Abraham, J.Q. Broughton, N. Bernstein and E. Kaxiras, *Computers in Physics* **12**, 538 (1998).
93. "A density functional study of clean and hydrogen-covered  $\alpha$ -MoO<sub>3</sub>(010): electronic structure and lattice relaxation", M. Chen, U.V. Waghmare, C.M. Friend and E. Kaxiras, *J. Chem. Phys.* **109**, 6854 (1998).
92. "Vacancy in silicon revisited: structure and pressure effects", A. Antonelli, E. Kaxiras and D.J. Chadi, *Phys. Rev. Lett.* **81**, 2088 (1998).

91. "Finite-temperature molecular-dynamics study of unstable stacking fault free energies in silicon", M. DeKoning, A. Antonelli, M.Z. Bazant, E. Kaxiras, J.F. Justo, *Phys. Rev. B* **58**, 12555 (1998).
90. "Effects of alloying on the ductility of MoSi<sub>2</sub> single crystals from first-principles calculations", U.V. Waghmare, E. Kaxiras, V. Bulatov and M.S. Duesbery, *Modelling Simul. Mater. Sci. Eng.* **6**, 483 (1998).
89. "Substitutional carbon impurities in thin silicon films: equilibrium structure and properties", P.C. Kelires and E. Kaxiras, *J. Vac. Sci. Technol. B* **16**, 1687 (1998).
88. "Amorphous-crystal interface in silicon: a tight-binding simulation", N. Bernstein, M.J. Aziz, E. Kaxiras, *Phys. Rev. B* **58**, 4579 (1998).
87. "Interatomic potential for silicon defects and disordered phases", J. F. Justo, M. Z. Bazant, E. Kaxiras, V. V. Bulatov, and S. Yip, *Phys. Rev. B* **58**, 2539 (1998).
86. "Diffusion of adsorbate atoms on the reconstructed Si(111) surface", K. Cho and E. Kaxiras, *Surf. Sci. Lett.* **396**, L261 (1998).
85. "Theory of adsorption and desorption of H<sub>2</sub> molecules on the Si(111)-(7 x 7) surface", K. Cho, E. Kaxiras and J.D. Joannopoulos, *Phys. Rev. Lett.* **79**, 5078 (1997).
84. "Surface reconstruction induced geometries of Si clusters", E. Kaxiras, *Phys. Rev. B* **56**, 13455 (1997).
83. "Non-orthogonal tight-binding Hamiltonians for defects and interfaces in silicon", N. Bernstein and E. Kaxiras, *Phys. Rev. B* **56**, 10488 (1997).
82. "Environment dependent interatomic potential for bulk silicon", M. Z. Bazant, E. Kaxiras and J. F. Justo, *Phys. Rev. B* **56**, 8542 (1997).
81. "Intermittent diffusion on the Si(111)(7 x 7) surface", K. Cho and E. Kaxiras, *Europhys. Lett.* **39**, 287 (1997).
80. "Semi-discrete variational Peierls framework for dislocation core properties", V. V. Bulatov and E. Kaxiras, *Phys. Rev. Lett.* **78**, 4221 (1997).
79. "Energetics and equilibrium properties of thin pseudomorphic Si<sub>1-x</sub>C<sub>x</sub>(100) layers in Si", P. C. Kelires and E. Kaxiras, *Phys. Rev. Lett.* **78**, 3479 (1997).
78. "Adaptive coordinate real-space electronic structure calculations for atoms, molecules and solids", N.A. Modine, G. Zumbach and E. Kaxiras, *Phys. Rev. B* **55**, 10289 (1997).
77. "Slip energy barriers in aluminium and implications for ductile versus brittle behaviour", Y. Sun and E. Kaxiras, *Phil. Mag. A* **75**, 1117 (1997).
76. "Simulations of structural materials", E. Kaxiras and J.R. Smith, *J. of Computer Aided Materials Design* **3**, 30 (1996).
75. "Modeling of covalent bonding in solids by inversion of cohesive energy curves", M. Z. Bazant and E. Kaxiras, *Phys. Rev. Lett.* **77**, 4370 (1996).
74. "Dynamic scaling in conserved systems with coupled fields: Application to surfactant mediated growth", A. L. Barabasi and E. Kaxiras, *Europhys. Lett.* **36**, 129 (1996).
73. "Generalized stacking fault energy surfaces and dislocation properties of silicon: a first-principles theoretical study", Y. Juan and E. Kaxiras, *Phil. Mag. A* **74**, 1367 (1996).
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71. "Review of atomistic simulations of surface diffusion and growth on semiconductors", E. Kaxiras, *Computational Materials Science* **6**, 158 (1996).
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11. “New classical potential for accurate simulation of atomic processes in Si”, E. Kaxiras and K.C. Pandey, *Phys. Rev. B* **38**, 12736 (1988).
10. “Energetics of defects and diffusion mechanisms in graphite”, E. Kaxiras and K.C. Pandey, *Phys. Rev. Lett.* **61**, 2693 (1988).
9. “Hole dynamics in the two-dimensional strong-coupling Hubbard Hamiltonian”, E. Kaxiras and E. Manousakis, *Phys. Rev. B* **38**, 866 (1988).
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### II.3 Conference Proceedings Articles:

22. “Metal sulfide and metal oxide nanostructures on Au(111): Synthesis and properties” C.M. Friend, J. Biener, M. Biener, D.H. Kang, H.Y. Deng, S.Y. Quek and E. Kaxiras, Abstracts of Am. Chem. Soc. **227**, U815 (2004).
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20. “First-principles and semiempirical electronic-structure calculations for single-stranded DNA”, D. Margetis, P. Maragakis, E. Kaxiras, M. Elstner and Th. Frauenheim, *Biophysical Journal* **80** (1), 488A (2001).
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16. “Unstable stacking fault free energies in silicon through empirical modeling”, M. De Koning, A. Antonelli, M.Z. Bazant, E. Kaxiras and J.F. Justo, MRS Symposium Proceedings, vol. 539, p. 175, edited by G.E. Beltz, R.L. Blumberg Selinger, K.-S. Kim, M.P. Marder (Materials Research Society, Pittsburgh, 1999).
15. “First-principles study of Si(111) homoepitaxy”, K. Cho and E. Kaxiras, MRS Symposium Proceedings, vol. 538, p. 341, edited by V. Bulatov, T.D. de la Rubia, N. Ghoniem, E. Kaxiras and R. Phillips (Materials Research Society, Pittsburgh, 1999).
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9. “Derivation of interatomic potentials by inversion of ab initio cohesive energy curves”, M. Z. Bazant and E. Kaxiras, MRS Symposium Proceedings, vol. 408, p. 79, edited by E. Kaxiras, J. Joannopoulos, P. Vashishta and R.K. Kalia (Materials Research Society, Pittsburgh, 1996).
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6. “Vibrational properties of silicon microclusters and comparison to the amorphous material”, J.L. Feldman and E. Kaxiras, MRS Symposium Proceedings vol. 206, p. 79, edited by R.S. Averback, J. Bernolc and D.N. Nelson (Materials Research Society, Pittsburgh, 1991).
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2. “Kinetics and growth channels in GaAs epitaxy on Si(100)”, O.L. Alerhand, E. Kaxiras, J.D. Joannopoulos and G.W. Turner, 20th International Conference on the Physics of Semiconductors, Proceedings vol. 1, p. 284, edited by E.M. Anastassakis and J.D. Joannopoulos (World Scientific, Singapore, 1990).
2. “A new classical potential for accurate total-energy calculations of atomic processes in Si”, E. Kaxiras and K.C. Pandey, 19th International Conference on the Physics of

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1. “Variable stoichiometry surface reconstruction: new models and phase transitions on GaAs<sub>111</sub>(2 x 2)”, E. Kaxiras, Y. Bar-Yam, J.D. Joannopoulos, K.C. Pandey, 18th International Conference on the Physics of Semiconductors, Proceedings vol. 1, p. 117, edited by O. Engstrom (World Scientific, Singapore, 1987).

### III. INVITED TALKS AT INTERNATIONAL CONFERENCES AND WORKSHOPS

94. “Multiscale simulations of complex materials for engineering and biological applications”, 11<sup>th</sup> International Conference on Phase Equilibria for Product and Process Design (20-25 May 2007, Hersonissos, Crete, Greece).
93. “Simulations of complex materials across multiple scales”, NanoMaterials for Defense Applications Symposium (23-26 April 2007, San Diego, California).
92. “Multiscale simulations of complex materials for engineering and biological applications”, 233<sup>rd</sup> Annual Meeting of the American Chemical Society (25-29 March 2007, Chicago, Illinois).
91. “Nanotube contacts with metal leads and DNA - from CNT-FETs to ultrafast sequencing”, Workshop on Simulations of Novel Carbon Materials, Centre Europeen de Calcul Atomique et Moleculaire - CECAM (25-28 October 2006, Lyon, France).
90. “Simulations of complex materials across multiple scales”, 19<sup>th</sup> Panhellenic Conference and Summer School on Nonlinear Science and Complexity (10-22 July 2006, Polytechnic School, Aristotle University of Thessaloniki, Greece).
89. “Simulations of complex materials across multiple scales”, 3<sup>rd</sup> Workshop on Nanosciences and Nanotechnologies (10-12 July 2006, Aristotle University of Thessaloniki, Greece).
88. “Hydrogen embrittlement of Aluminum: first-principles calculations and multiscale simulations”, Symposium on Micro- and Nano-mechanics of Structural Materials, Fall Meeting of Materials Research Society (28 November – 3 December 2005, Boston, Massachusetts).
87. **(Keynote)** “Multiscale models for complex materials: mechanochemistry, DNA and CNT nanowires, ATP-synthase function”, Topical Conference on Multiscale Analysis in Chemical, Materials and Biological Processes, Annual Meeting of American Institute of Chemical Engineers (30 October – 4 November 2005, Cincinnati, Ohio).
86. “A new class of semiconducting nanotubes based on metal-cyanide complexes”, Workshop on Computational Materials and Molecular Electronics, Institute for Computational Engineering and Sciences, University of Texas, Austin (20-22 October 2005, Austin, Texas).
85. “Multiscale modeling of materials”, Workshop on Multiscale Modeling in Condensed Matter and Materials Sciences, Institute for Pure and Applied Mathematics, University of California, Los Angeles (17-20 October 2005, Los Angeles, California).
84. “Multiscale modeling and growth phenomena on surfaces”, Workshop on Multiscale Studies of Formation and Stability of Surface-based Nanostructures, University of Wisconsin (14-15 October 2005, Madison, Wisconsin).

83. **(Hot Topics)** “Tuning the wettability of surfaces from hydrophobic to super-hydrophilic by submonolayer chemical modification: the case of X-C(111), X=Li, Na, K”, Gordon Research Conference on Thin Film and Crystal Growth Mechanisms (26-30 June 2005, Mount Holyoke College, South Hadley, Massachusetts).
82. **(Keynote)** “Multiscale modeling of materials: Application to mechano-chemistry of metals”, Symposium on Multiscale Modeling of Materials Behavior – Solids, Third M.I.T. Conference on Computational Fluid and Solid Mechanics (14-17 June 2005, Cambridge, Massachusetts).
81. “Multiscale Simulation of Materials: from Covalent to Metallic Bonding, Tests and Applications”, Workshop on Multiscale Modeling in Solids, 2004-2005 Theme Year on Mathematics of Stochastic and Multiscale Modeling, Centre de Reserches Mathematiques, Universite de Montreal (28-30 April 2005, Montreal, Canada).
80. “Multiscale Simulation of Materials: from Covalent to Metallic Bonding, Tests and Applications”, Symposium on Linking Length Scales in Mechanical Behavior of Materials, Spring Meeting of the Materials Research Society (29-31 March 2005, San Francisco, California).
79. “Contrasting growth modes of Mn on Ge(100) and Ge(111) surfaces: Subsurfactant action versus intermixing”, Second International Conference on Multiscale Materials Modeling, (11-15 October 2004, UCLA-Los Angeles, California).
78. “Multiscale Simulations in Materials Science”, European Conference on Computational Physics, (1-4 September 2004, Genoa, Italy).
77. “Simulations of Complex Systems Across Scales: Connecting the Nano to the Macro World”, Indo-US Workshop on Nanotechnology: Issues in Interdisciplinary Research and Education (11-13 August 2004, Bangalore, India).
76. “The Nanotechnology Revolution: the Role and Necessity of Theory and Simulations”, The Onassis Lectures on Chemistry and Physics, Foundation for Research and Technology-Hellas (19-23 July 2004, Heraklion, Crete, Greece).
75. “Coupling of Scales in Simulations of Mechanical Behavior of Metals with Chemical Impurities”, March Meeting of the American Physical Society (22-26 March 2004, Montreal, Canada).
74. “Multiscale Modelling of Complex Physical Systems”, 13<sup>th</sup> Microelectronics Workshop, National Center for Scientific Research Demokritos (4 – 6 February 2004, Athens, Greece).
73. “Real-space Multiscale Simulations for Metals: Implementation of Density-functional with Embedded Atom Coupling”, Symposium on Atomic Scale Materials Design Modeling and Simulation, Fall Meeting of Materials Research Society (1 - 5 December 2003, Boston, Massachusetts).
72. “Multiscale modeling of complex physical systems”, XIX Panhellenic Conference on Condensed Matter Physics, Aristotle University of Thessaloniki (21 - 24 September 2003, Thessaloniki, Greece).
71. “Modeling complex physical systems across length scales: progress and problems”, Schloss Ringberg Conference on Modeling Statistics and Dynamics in Catalysis: from *ab initio* potentials to rare events (10 - 13 September 2003, Munich, Germany).
70. **(Plenary)** “Simulations of complex systems across multiple length scales”, Second MIT Conference on Computational Fluid and Solid Mechanics, Massachusetts Institute of Technology (17 - 20 June 2003, Cambridge, Massachusetts).

69. “Multiscale modeling of complex physical systems”, Conference on Frontiers in Materials and Nanoscience: Novel Phenomena and New Structures, Harvard Engineering and Applied Sciences Industrial Outreach Program, Harvard University (10 - 11 April 2003, Cambridge, Massachusetts).
68. “Simulations of complex systems across multiple length scales”, NANO-2002 Workshop IV: Modeling and Simulation of Materials, Institute of Pure and Applied Mathematics, University of California, Los Angeles (19 - 22 November 2002, Los Angeles, California).
67. **(Plenary)** “Multiscale modeling of complex phenomena involving chemical interactions”, Sixth World Congress of Theoretically Oriented Chemists (4 - 9 August 2002, Lugano, Switzerland).
66. “Multiscale simulations of the behavior of solids under extreme loads”, Frontiers in Information Technology Symposium, Rensselaer Polytechnic Institute (8 November 2001, Troy, New York).
65. “Multiscale simulations of the behavior of solids under extreme loads”, Second International Conference on Multiscale Modeling, The Knowledge Foundation (13 - 14 August 2001, Boston, Massachusetts).
64. “Multiscale approaches based on ab initio calculations”, Thirteenth Annual Workshop on Recent Developments in Electronic Structure Algorithms, Princeton University (15 - 18 June 2001, Princeton, New Jersey).
63. “Multiscale simulations of deformations of solids under external loading”, Symposium on Multiscale Materials Modeling, Fall Meeting of Materials Research Society (27 November - 1 December 2000, Boston, Massachusetts).
62. “Bulk and surface structure of amorphous silicon”, International Symposium on Wave Propagation and Electronic Structure of Disordered Systems, Foundation for Research and Technology - Hellas (15 - 17 June 2000, Heraklion, Crete, Greece).
61. “Bulk and surface structure of amorphous silicon”, Workshop on Electronic and Optical Properties of Semiconducting Glasses, Centre Europeen pour le Calcul Atomique et Moleculaire (13 - 16 June 2000, Lyon, France).
60. “Quantum to atomistic coupling in multiscale modeling”, Workshop on Multiscale Modeling of Materials (17 - 19 May 2000, Newport, Rhode Island).
59. “Quantum mechanical simulations of chemical reactions in high-stress and high-pressure environments in solids”, Symposium on Physical Chemistry at High Pressure and Temperature, National Meeting of the American Chemical Society (26 - 30 March 2000, San Francisco, California).
58. “Multiscale modeling of materials properties”, ONR Workshop on Grand Challenges: Materials by Design (6 - 7 January 2000, Alexandria, Virginia).
57. “Multiscale modeling of materials”, Symposium on Nanomechanics of Surfaces and Interfaces, Annual Meeting of the Society of Engineering Science (25 - 27 October 1999, Austin, Texas).
56. “Multiscale modeling of brittle materials”, NIST Workshop on Hybrid Methods in Multiscale Modeling of Materials (12 - 14 May 1999, Gaithersburg, Maryland).
55. “From the microscopic structure of semiconductors to their macroscopic electronic and mechanical properties”, Ninth Brazilian Workshop on Semiconductor Physics (7 - 12 February 1999, Bello Horizonte, Brazil).
54. “Applications of first-principles and empirical methods in determining activated states at surfaces and interfaces of silicon”, Symposium on Computation of Rates of Activated

- Processes, Fall Meeting of Materials Research Society (30 November - 2 December 1998, Boston, Massachusetts).
53. "From the electronic structure of solids to the macroscopic behavior of materials", Workshop on Opportunities in Materials Theory, National Science Foundation (8 - 9 October 1998, Arlington, Virginia).
  52. "Development and applications of empirical and semi-empirical methods to the study of disordered covalent systems", Workshop on Local Orbital Methods for Large Scale Atomistic Simulations, Centre Europeen pour le Calcul Atomique et Moleculaire (22 - 25 July 1998, Lyon, France).
  51. "From microscopic atomic motion to macroscopic properties of solids using first-principles calculations", March Meeting of the American Physical Society (16 - 20 March 1998, Los Angeles, California).
  50. "First-principles studies of the structure of III-V surfaces under growth conditions", Virtual Integrated Prototyping Workshop, California Institute of Technology (27 - 28 January, 1998, Pasadena, California).
  49. "Theory of diffusion and growth phenomena on semiconductor surfaces", 25th Conference on the Physics and Chemistry of Semiconductor Interfaces (19 - 22 January 1998, Salt Lake City, Utah).
  48. "Theoretical studies of atomic structure and dynamics on semiconductor surfaces and interfaces", Symposium on Microscopic Simulation of Interfacial Phenomena in Solids and Liquids, Fall Meeting of Materials Research Society (1 - 5 December 1997, Boston, Massachusetts).
  47. "Atomistic studies of macroscopic behavior of materials", Workshop on Linking of Scales from Atomistic to Continuum, Centre Europeen pour le Calcul Atomique et Moleculaire (20 - 22 October 1997, Lyon, France).
  46. "Ab-initio simulations: an unexplored resource for modeling", Challenges in Predictive Process Simulation Workshop (17 - 20 August 1997, Wandlitz, Germany).
  45. "Diffusion and Growth Phenomena on Semiconductor Surfaces: from Microscopic Mechanisms to Morphological Instabilities", Fifteenth Conference on Crystal Growth and Epitaxy, American Association for Crystal Growth (1 - 4 June 1997, Fallen Leaf Lake, California).
  44. "Diffusion and growth phenomena on semiconductor surfaces", Symposium on Computational Methods for Materials Science, Molecular Simulations Inc. (25 April 1997, San Diego, California).
  43. "Theoretical studies of microscopic mechanisms of diffusion and growth on semiconductors", Symposium on New Concepts in Surface Chemistry: Diffusive Motion of Atoms and Molecules on Surfaces, 213th National Meeting of the American Chemical Society (13 - 17 April 1997, San Francisco, California).
  42. "Growth phenomena on semiconductor surfaces: from atomic diffusion to the formation of nanostructures", International Symposium on Novel Materials (3 - 7 March 1997, Puri, India).
  41. "Theoretical studies of diffusion and growth phenomena on semiconductor surfaces" 43rd National Symposium of the American Vacuum Society (14 - 18 October 1996, Philadelphia, Pennsylvania).
  40. "Theory of atom dynamics on semiconductors: from diffusion to growth", Conference on Crystal Surfaces and Interfaces (4 - 8 August 1996, Traverse City, Michigan).

39. “Adaptive coordinates real-space electronic structure: fundamentals and basic issues”, Workshop on Grid, Multigrid and Wavelet Methods in Electronic Structure Calculations, Centre Europeen pour le Calcul Atomique et Moleculaire (4 - 6 July 1996, Lyon, France).
38. “Theory of diffusion and growth phenomena, using first-principles results and stochastic simulations”, International Workshop on First-principle, Tight-binding and Empirical Methods for Materials Simulation, Institut für Physik, Technische Universität Chemnitz (26 - 29 June 1996, Chemnitz, Germany).
37. “Diffusion and growth on semiconductor surfaces”, Sixth Conference on Computational Research on Materials, West Virginia University (8 - 10 May 1996, Morgantown, West Virginia).
36. “The study of diffusion and growth phenomena using electronic structure calculations”, March Meeting of the American Physical Society (18 - 22 March 1996, St. Louis, Missouri).
35. “Theoretical studies of diffusion and growth phenomena on semiconductor surfaces”, Mardi Gras Conference on Experimental and Simulation Challenges in Nanostructured Materials, Louisiana State University (15 - 17 February 1996, Baton Rouge, Louisiana).
34. “Theoretical studies of diffusion and growth phenomena on semiconductor surfaces”, Workshop on Modeling of Industrial Materials: Connecting the Atomistic and Continuum Scales, Institute for Theoretical Physics, University of California Santa Barbara (7 - 11 January 1996, Santa Barbara, California).
33. “Microscopic theory of dynamical phenomena: diffusion and growth on semiconductor surfaces”, Materials Modeling 95 Workshop, Naval Research Laboratory (17 - 18 October 1995, Washington, DC).
32. “Microscopic theory of diffusion and growth on semiconductor surfaces”, International Symposium on Si Heterostructures: from Physics to Devices (11 - 14 September 1995, Heraklion, Greece).
31. “Diffusion on realistic semiconductor surfaces: the vagaries of surface reconstruction”; “Surfactant mediated growth on semiconductor surfaces: models for homoepitaxy and heteroepitaxy”, Workshop on Computer Simulations of Crystal and Overlayer Growth, Centre Europeen pour le Calcul Atomique et Moleculaire (28 August - 8 September 1995, Lyon, France).
30. “Theoretical studies of surface diffusion and growth of semiconductors”, International Conference on Surface Science: Critical Review and Outlook, University of Hong Kong (19 - 23 June 1995, Hong Kong).
29. “Review of atomistic models used in understanding semiconductor growth”, Virtual Molecular Beam Epitaxy Workshop, Hughes Research Laboratories (15 - 17 June 1995, Malibu, California).
28. “First-principles calculations and simulations of diffusion and growth on semiconductor surfaces”, ARPA Workshop on Vapor Phase Process Modeling (2 - 3 May 1995, Charlottesville, Virginia).
27. “Recent first-principles results for generalized stacking fault theory of silicon and aluminum”, NIST Workshop on Mechanics and Atomistics of Mechanical Behavior (27 - 28 April 1995, Gaithersburg, Maryland).
26. “First-principles calculations and simulations of diffusion and growth on semiconductor surfaces”, 31st Annual Symposium of the New Mexico Chapter of the American Vacuum Society (10 - 14 April 1995, Albuquerque, New Mexico).

25. “Energetics of generalized stacking faults and dislocation dynamics in silicon”, Adriatico Research Conference on Lower Dimensionality Semiconductor Systems, University of Campinas (20 - 24 February 1995, Campinas, Brazil).
24. “Theoretical studies of diffusion and growth on semiconductor surfaces”, Theoretical and Experimental Workshop on the Physics of Semiconductor Microstructures, University of Campinas (13 - 24 February 1995, Campinas, Brazil).
23. “Dynamics of atoms on surfaces, interfaces and defects of solids, based on first-principles calculations”, Symposium on Computational Approaches and Applications to Predicting the Properties of Complex Materials, Fall Meeting of the Materials Research Society (28 November - 2 December 1994, Boston, Massachusetts).
22. “Dynamics of atoms on surfaces and in bulk solids, based on first-principles calculations”, European Research Conference on Electronic Structure of Solids (27 August - 1 September 1994, Gausdal, Norway).
21. “Theoretical studies of surface and sub-surface diffusion”, Workshop on Critical Issues in Epitaxy, Electronic Materials Conference, University of Colorado (22-24 June 1994, Boulder, Colorado).
20. “First-principles calculations and classical simulations of surfactant mediated growth on semiconductor surfaces”, Workshop on Computer Simulation of the Growth of Semiconductor Materials, Centre Europeen pour le Calcul Atomique et Moleculaire (30 May - 2 June 1994, Lyon, France).
19. “Applications of first-principles calculations to dynamical processes in solids”, Workshop on Computational Methods for the Structure and Dynamics of Solids, Center for Computational Sciences, University of Kentucky (23-25 May 1994, Lexington, Kentucky).
18. “Energetics of generalized stacking faults in Si and relation to dislocation dynamics”, Symposium on Theory and Simulation of Time-Dependent Properties of Materials, Spring Meeting of the Materials Research Society (4-8 April 1994, San Francisco, California).
17. “Interplay of strain and chemical bonding on semiconductor surfaces: effects on atomic structure, diffusion and growth”, Sixth Annual Conference of National Alliance of Research Centers of Excellence, Center for Theoretical Studies of Physical Systems, Clark-Atlanta University (17-19 March 1994, Atlanta, Georgia).
16. “Theoretical studies of atomic structure and dynamics of thin films on semiconductor surfaces”, Gordon Research Conference on Chemistry of Electronic Materials (6-11 March 1994, Ventura, California).
15. “Surface diffusion and epitaxial layer-by-layer growth”, Workshop on Dynamics of Surface Growth, Vanderbilt University (28-30 October 1993, Nashville, Tennessee).
14. “The role of first-principles calculations in materials interfaces”, Workshop on Microstructure Formation and Evolution in Thin Films, IBM T.J. Watson Research Center (25-27 October 1993, Ossining, New York).
13. “Structure and properties of intermediate-size clusters of silicon and carbon”, First International Symposium on Theory of Atomic and Molecular Clusters, University of Oldenburg (13-18 June 1993, Leer, Germany).
12. “The use of quantum-mechanical calculations in dislocation structure and dynamics”, Workshop on Materials Computation: Dislocation Dynamics, Advanced Research Projects Agency (24-25 May 1993, Arlington, Virginia).

11. "First-principles thermodynamics of atomic motion and structural transformations in solids", Symposium on Computational Physics, March Meeting of the American Physical Society (22-26 March 1993, Seattle, Washington).
10. "Free-energies of generalized stacking faults in Si and the brittle-to-ductile transition", Workshop on Mechanics and Atomistics of Mechanical Behavior Institute for Theoretical Physics, University of California Santa Barbara (12 - 14 January 1993, Santa Barbara, California).
9. "Interplay of strain and chemical bonding on semiconductor surfaces", Symposium on Materials Theory and Modeling, Fall Meeting of the Materials Research Society (30 November - 4 December 1992, Boston, Massachusetts).
8. "Theoretical modeling of heteroepitaxial growth initiation", Workshop on Epitaxy, Interfaces, Defects and Processing of Electronic and Photonic Materials, Carnegie-Mellon University (4-8 November 1991, Pittsburgh, Pennsylvania).
7. "Strain and electronic energies in growth initiation", Gordon Research Conference on Inorganic Interfaces and Thin Films (8-12 July 1991, Plymouth, New Hampshire).
6. "Early stages of growth of GaAs on Si(100)", Symposium on Dissimilar Materials, Spring Meeting of the Materials Research Society (29 April-3 May 1991, Anaheim, California).
5. "Structure and electronic properties of semiconductor interfaces", Twentieth International Conference on the Physics of Semiconductors (5-10 August 1990, Thessaloniki, Greece).
4. "Microscopic theory of GaAs growth on vicinal Si(100) surfaces", Second International Symposium on Process Physics and Modeling in Semiconductor Technology, Spring Meeting of the Electrochemical Society (6-11 May 1990, Montreal, Canada).
3. "A new classical potential for accurate total-energy calculations of atomic processes in Si", Fourth International Workshop on Computational Condensed Matter Physics: Total Energy and Force Methods, International Center for Theoretical Physics (4-6 January 1989, Trieste, Italy).
2. "Polar surfaces of semiconductors", Symposium on Surfaces and Interfaces: Treatment, Modifications, Applications and Characterization, Massachusetts Institute of Technology (21-22 May 1988, Cambridge, Massachusetts).
1. "Variable stoichiometry surface reconstruction: New models and phase transitions on GaAs {111}(2 x 2)", March Meeting of the American Physical Society (March 1987, New York, New York).