

Recent Publications from the NTI

Morelos-Gómez, A.; Vega-Díaz, S. M.; González, V. J.; Tristán-López, F.; Cruz-Silva, R.; Fujisawa, K.; Muramatsu, H.; Hayashi, T.; Mi, X.; Shi, Y.; Sakamoto, H.; Khoerunnisa, F.; Kaneko, K.; Sumpter, B. G.; Kim, Y. A.; Meunier, V.; Endo, M.; Muñoz-Sandoval, E.; Terrones, M., "Clean Nanotube Unzipping by Abrupt Thermal Expansion of Molecular Nitrogen: Graphene Nanoribbons with Atomically Smooth Edges" *ACS Nano* **6** (3), 2261–2272 (2012).

Šponer, J. E.; Mladek, A.; Šponer, J.; Fuentes-Cabrera, M., "Formamide-Based Prebiotic Synthesis of Nucleobases: A Kinetically Accessible Reaction Route," *J. Phys. Chem. A* **116** (1), 720–726 (2012).

Sumpter, B. G.; Meunier, V., "Can Computational Approaches Aid in Untangling the Inherent Complexity of Practical Organic Photovoltaic Systems?" *J. Polym. Sci., Part B: Polym. Phys.* **50** (15), 1071–1089 (2012).

Sun, C. H.; Liao, T.; Lu, G. Q.; Smith, S. C., "The Role of Atomic Vacancy on Water Dissociation over Titanium Dioxide Nanosheet: A Density Functional Theory Study," *J. Phys. Chem. C* **116** (3), 2477–2482 (2012).

Wang, S. G.; Ward, R.C.C.; Hesjedal, T.; Zhang, X. G.; Wang, C.; Kohn, A.; Ma, Q. L.; Zhang, J.; Liu, H. F.; Han, X. F., "Interface Characterization of Epitaxial Fe/MgO/Fe Magnetic Tunnel Junctions," *J. Nanosci. Nanotechnol.* **12** (2), 1006–1023 (2012).

Wang, X. J.; Goswami, M.; Kumar, R.; Sumpter, B. G.; Mays, J., "Morphologies of Block Copolymers Composed of Charged and Neutral Blocks," *Soft Matter* **8** (11), 3036–3052 (2012).

Wu, P.; Huang, J. S.; Meunier, V.; Sumpter, B. G.; Qiao, R., "Voltage Dependent Charge Storage Modes and Capacity in Subnanometer Pores," *J. Phys. Chem. Lett.* **3** (13), 1732–1737 (2012).

Zhang, J.; Zhang, X. -G.; Han, X. F., "Spinel Oxides: Δ_1 Spin-Filter Barrier For a Class of Magnetic Tunnel Junctions," *Appl. Phys. Lett.* **100** (22), 222401 (2012).

Zhang, X.-G.; Xiang, T., "Tunable Coulomb Blockade and Giant Coulomb Blockade Magnetoresistance in a Double Quantum Dot System," *Int. J. Quantum Chem.* **112** (1), 28–32 (2012).

Buenzli, P. R.; Jeon, J.; Pivonka, P.; Smith, D. W.; Cummings, P.T., "Investigation of Bone Resorption Within a Cortical Basic Multicellular Unit Using a Lattice-Based Computational Model," *Bone* **50** (1), 378–389 (2012).

Chen, J.; Yu, X.; Hong, K. L.; Messman, J. M.; Pickel, D. L.; Xiao, K.; Dadmun, M. D.; Mays, J. W.; Rondinone, A. J.; Sumpter, B. G.; Kilbey, II., S. M., "Ternary Behavior and Systematic Nanoscale Manipulation of Domain Structures in P2HT/PCBM/P2HT-*b*-PEO Films," *J. Mater. Chem.* **22** (26), 13013–13022 (2012).

Clark, K. W.; Qin, S. Y.; Zhang, X. G.; Li, A. P., "Nanoscale Periodic Modulations on Sodium Chloride Surface Revealed by Tuning Fork Atomic Force Microscopy," *Nanotechnology* **23** (18), 185306 (2012).

Du, A. J.; Sanvito, S.; Smith, S. C., "First-Principles Prediction of Metal-Free Magnetism and Intrinsic Half-Metallicity in Graphitic Carbon Nitride," *Phys. Rev. Lett.* **108** (19), 197207 (2012).

Ehemann, R. C.; Krstic, P. S.; Dadras, J.; Kent, P.R.C.; Jakowski, J., "Detection of Hydrogen Using Graphene," *Nanoscale Res. Lett.* **7**, 1–14 (2012).

Friemel, G.; Park, J. T.; Maier, T. A.; Tsurkan, V.; Li, Y.; Deisenhofer, J.; von Nidda, H.A.K.; Loidl, A.; Ivanov, A.; Keimer, B.; Inosov, D. S., "Reciprocal-Space Structure and Dispersion of the Magnetic Resonant Mode in the Superconducting Phase of $Rb_xFe_{2-y}Se_2$ Single Crystals," *Phys. Rev. B* **85** (14), 140511 (2012).

Gai, Z.; Zhang, X.-G.; Kravchenko, I. I.; Retterer, S. T.; Wendelken, J. F., "Quenching of Initial ac Susceptibility in Single-Domain Ni Nanobars," *Phys. Rev. B* **85** (2), 024401 (2012).

Hankel, M.; Jiao, Y.; Du, A. J.; Gray, S. K.; Smith, S. C., "Asymmetrically Decorated, Doped Porous Graphene as an Effective Membrane for Hydrogen Isotope Separation," *J. Phys. Chem. C* **116** (11), 6672–6676 (2012).

Liao, T.; Sun, C. H.; Du, A. J.; Sun, Z. Q.; Hulicova-Jurcakova, D.; Smith, S., "Charge Carrier Exchange at Chemically Modified Graphene Edges: A Density Functional Theory Study," *J. Mater. Chem.* **22** (17), 8321–8326 (2012).

Hashim, D. P.; Narayanan, N. T.; Romo-Herrera, J. M.; Cullen, D. A.; Hahm, M. G.; Lezzi, P.; Suttle, J. R.; Kelkhoff, D.; Munoz-Sandoval, E.; Ganguli, S.; Roy, A. K.; Smith, D. J.; Vajtai, R.; Sumpter, B. G.; Meunier, V.; Terrones, H.; Terrones, M.; Ajayan, P. M., "Covalently Bonded Three-Dimensional Carbon Nanotube Solids via Boron Induced Nanojunctions," *Sci. Rep.* **2**, 363 (2012).

Heredia, A.; Meunier, V.; Bdikin, I. K.; Gracio, J.; Balke, N.; Jesse, S.; Tselev, A.; Agarwal, P. K.; Sumpter, B. G.; Kalinin, S. V.; Khoklin, A. L., "Nanoscale Ferroelectricity in Crystalline γ -Glycine," *Adv. Funct. Mater.* **22** (14), 2996–3003 (2012).

Jakowski, J.; Irle, S.; Sumpter, B. G.; Morokuma, K., "Modeling Charge Transfer in Fullerene Collisions via Real-Time Electron Dynamics," *J. Phys. Chem. Lett.* **3** (11), 1536–1542 (2012).

Kumar, R.; Sumpter, B. G.; Kilbey, II, S. M., "Charge Regulation and Local Dielectric Function in Planar Polyelectrolyte Brushes," *J. Chem. Phys.* **136** (23), 234901 (2012).

Li, Q.; Han, C. B.; Horton, S. R.; Fuentes-Cabrera, M.; Sumpter, B. G.; Lu, W. C.; Bernholc, J.; Maksymovych, P.; Pan, M. H., "Supramolecular Self-Assembly of π -Conjugated Hydrocarbons via 2D Cooperative CH/ π Interaction," *ACS Nano* **6** (1), 566–572 (2012).

Alonzo, J.; Chen, J.; Messman, J.; Yu, Z.; Hong, K.; Deng, S.; Swader, O.; Dadmun, M.; Ankner, J. F.; Britt, P.; Mays, J. W.; Malagoli, M.; Sumpter, B. G.; Bredas, J.-L.; Kilbey, II, S. M., "Assembly and Characterization of Well-Defined High-Molecular-Weight Poly(*p*-phenylene) Polymer Brushes," *Chem. Mater.* **23** (19), 4367–4374 (2011).

An, J. M.; Barabash, S. V.; Ozolins, V.; van Schilfgaard, M.; Belashchenko, K. D.; "First-Principles Study of Phase Stability of Gd-Doped EuO and EuS," *Phys. Rev. B* **83** 064105 (2011).

Bajdich, M.; Kent, P.R.C.; Kim, J.; Reboreda, F. A., "Simple Impurity Embedded in a Spherical Jellium: Approximations of Density Functional Theory Compared to Quantum Monte Carlo Benchmarks," *Phys. Rev. B* **84** (7), 075131 (2011).

Blas, J. R.; Huertas, O.; Tabares, C.; Sumpter, B. G.; Fuentes-Cabrera, M.; Orozco, M.; Ordejón, P.; Luque, F. J., "Structural, Dynamical, and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases," *J. Phys. Chem. A* **115** (41), 11344–11354 (2011).

Botello-Méndez, A. R.; Cruz-Silva, E.; Romo-Herrera, J. M.; Lopez-Urias, F.; Terrones, M.; Sumpter, B. G.; Terrones, H.; Charlier, J.-C.; Meunier, V., "Quantum Transport in Graphene Nanonetworks," *Nano Lett.* **11** (8), 3058–3064 (2011).

Burns, L. A.; Vazquez-Mayagoitia, A.; Sumpter, B. G.; Sherrill, C. D., "Density-Functional Approaches to Noncovalent Interactions: A Comparison of Dispersion Corrections (DFT-D), Exchange-Hole Dipole Moment (XDM) Theory, and Specialized Functionals," *J. Chem. Phys.* **134** (8), 084107 (2011).

Campbell, K.; Gurun, B.; Sumpter, B. G.; Thio, Y. S.; Bucknall, D. G., "Role of Conformation in π - π Interactions and Polymer/Fullerene Miscibility," *J. Phys. Chem. B* **115** (29), 8989–8995 (2011).

Cao, C.; Wang, Y.; Cheng, H.-P.; Jiang, J. Z., "Perfect Spin-Filtering and Giant Magnetoresistance with Fe-Terminated Graphene Nanoribbon," *Appl. Phys. Lett.* **99** (7), 073110 (2011).

Chen, Y. -W.; Chu, I. -H.; Wang, Y.; Cheng, H. -P., "Water Thin Film-Silica Interaction on α -Quartz (0001) Surfaces," *Phys. Rev. B* **84** (15), 155444 (2011).

Chu, I. -H.; Radulaski, M.; Vukmirovic, N.; Cheng, H. -P.; Wang, L. -W., "Charge Transport in a Quantum Dot Supercrystal," *J. Phys. Chem. C* **115** (43), 21409–21415 (2011).

Cruz-Silva, E.; Barnett, Z. M.; Sumpter, B. G.; Meunier, V., "Structural, Magnetic, and Transport Properties of Substitutionally Doped Graphene Nanoribbons From First

Principles" *Phys. Rev. B* **83**, 155445 (2011).

Cruz-Silva, E.; Lopez-Urias, F.; Muñoz-Sandoval, E.; Sumpter, B. G.; Terrones, H.; Charlier, J.-C.; Meunier, V.; Terrones, M., "Phosphorus and Phosphorus-Nitrogen Doped Carbon Nanotubes for Ultrasensitive and Selective Molecular Detection," *Nanoscale* **3** (3), 1008–1013 (2011).

Delaire, O.; Marty, K.; Stone, M. B.; Kent, P.R.C.; Lucas, M. S.; Abernathy, D. L.; Mandrus, D.; Sales, B. C., "Phonon Softening and Metallization of a Narrow-Gap Semiconductor by Thermal Disorder," *Proc. Nat. Acad. Sci.* **108** (12), 4725–4730 (2011).

Feng, G.; Huang, J.-S.; Sumpter, B. G.; Meunier, V.; Qiao, R., "A 'Counter-Charge layer in Generalized Solvents' Framework for Electrical Double Layers in Neat and Hybrid Ionic Liquid Electrolytes," *Phys. Chem. Chem. Phys.* **13** (32), 14723–14734 (2011).

Feng, G.; Qiao, R.; Huang, J. S.; Dai, S.; Sumpter, B. G.; Meunier, V., "The Importance of Ion Size and Electrode Curvature on Electrical Double Layers in Ionic Liquids," *Phys. Chem. Chem. Phys.* **13** (3), 1152–1161 (2011).

Fuentes-Cabrera, M.; Rhodes, B. H.; Fowlkes, J. D.; Lopez-Benzanilla, A.; Terrones, H.; Simpson, M. L.; Rack, P. D., "Molecular Dynamics Study of the Dewetting of Copper on Graphite and Graphene: Implications for Nanoscale Self-Assembly," *Phys. Rev. E* **83** (4), 041603 (2011).

Gonis, A.; Zhang, X. G.; Nicholson, D. M.; Stocks, G. M., "Antisymmetric Wave Functions For Mixed Fermion States and Energy Convexity," *Phys. Rev. B* **84** (4), 045121 (2011).

Gull, E.; Staar, P.; Fuchs, S.; Nukala, P.; Summers, M. S.; Pruschke, T.; Schulthess, T. C.; Maier, T., "Submatrix Updates for the Continuous-Time Auxiliary-Field Algorithm," *Phys. Rev. B* **83** (7), 075122 (2011).

Huang, J. S.; Sumpter, B. G.; Meunier, V.; Tian, Y. H.; Kertesz, M., "Cyclo-Biphenalenyl Biradicaloid Molecular Materials: Conformation, Tautomerization, Magnetism, and Thermochromism," *Chem. Mater.* **23** (3), 874–885 (2011).

Iacovella, C. R.; French, W. R.; Cook, B. G.; Kent, P.R.C.; Cummings, P. T., "Role of Polytetrahedral Structures in the Elongation and Rupture of Gold Nanowires," *ACS Nano* **5** (12), 10065–10073 (2011).

Kemper, A. F.; Korshunov, M. M.; Devvereaux, T. P.; Fry, J. N.; Cheng, H. -P.; Hirschfeld, P. J., "Anisotropic Quasiparticle Lifetimes in Fe-Based Superconductors," *Phys. Rev. B* **83** (18), 184516 (2011).

Kent, P.R.C.; Dadras, J.; Krstic, P. S., "Improved Hydrocarbon Potentials for Sputtering Studies," *J. Nucl. Mater.* **415** (1), S183–S186 (2011).

Kim, T. H.; Nicholson, D. M.; Zhang, X. G.; Evans, B. M.; Kulkarni, N. S.; Kenik, E. A.; Meyer, H. M.; Radhakrishnan, B.; Li, A. P., "Structural Dependence of Grain Boundary Resistivity in Copper Nanowires," *Jpn. J. Appl. Phys.* **50** (8), 08LB09 (2011).

Kumar, N.; Kent, P.R.C.; Bandura, A. V.; Kubicki, J. D.; Wesolowski, D. J.; Cole, D. R.; Sofo, J. O., "Faster Proton Transfer Dynamics of Water on SnO₂ Compared to TiO₂," *J. Chem. Phys.* **134** (4), 044706 (2011).

Labastide, J. A.; Baghgar, M.; Dujovne, I.; Yang, Y.; Dinsmore, A. D.; Sumpter, B. G.; Venkataraman, D.; Barnes, M. D., "Polymer Nanoparticle Superlattices for Organic Photovoltaic Applications," *J. Phys. Chem. Lett.* **2** (24), 3085–3091 (2011).

Lopez-Bezanilla, A.; Huang, J.; Terrones, H.; Sumpter, B. G., "Boron Nitride Nanoribbons Become Metallic," *Nano Lett.* **11** (8), 3267–3273 (2011).

Ma, Q. L.; Wang, S. G.; Wei, H. X.; Liu, H. F.; Zhang, X. G.; Han, X. F., "Evidence for Magnon Excitation Contribution to the Magnetoresistance Behavior During Thermal Annealing in CoFeB/MgO/CoFeB Magnetic Tunnel Junctions," *Phys. Rev. B* **83** (22), 224430 (2011).

Maier, T. A.; Graser, S.; Hirschfeld, P. J.; Scalapino, D. J., "d-Wave Pairing From Spin Fluctuations in the K_xFe_{2-y}Se₂ Superconductors," *Phys. Rev. B* **83** (10), 100515 (2011).

Maier, T. A.; Graser, S.; Hirschfeld, P. J.; Scalapino, D. J., "Inelastic Neutron and X-Ray Scattering as Probes of the Sign Structure of the Superconducting Gap in Iron Pnictides," *Phys. Rev. B* **83** (22), 220505 (2011).

Maier, T.; Scalapino, D., "Pair Structure and the Pairing Interaction in a Bilayer Hubbard Model for Unconventional Superconductivity," *Phys. Rev. B* **84** (18), 180513 (2011).

Maiti, S.; Korshunov, M. M.; Maier, T. A.; Hirschfeld, P. J.; Chubukov, A. V., "Evolution of Symmetry and Structure of the Gap in Iron-Based Superconductors with Doping and Interactions," *Phys. Rev. B* **84** (22), 224505 (2011).

Maiti, S.; Korshunov, M. M.; Maier, T. A.; Hirschfeld, P. J.; Chubukov, A. V., "Evolution of the Superconducting State of Fe-Based Compounds with Doping," *Phys. Rev. Lett.* **107** (14), 147002 (2011).

Messman, J. M.; Pickel, D. L.; Goswami, M.; Uhrig, D. W.; Sumpter, B. G.; Mays, J. W., "Combatting Ionic Aggregation Using Dielectric Forces-Combining Modeling/Simulation and Experimental Results to Explain End-Capping of Primary Amine Functionalized Polystyrene," *Polym. Chem.* **2** (11), 2481–2489 (2011).

Mladek, A.; Šponer, J.; Sumpter, B. G.; Fuentes-Cabrera, M.; Šponer, J. E., "On the Geometry and Electronic Structure of the As-DNA Backbone," *J. Phys. Chem. Lett.* **2** (5), 389–392 (2011).

Mladek, A.; Šponer, J.; Sumpter, B. G.; Fuentes-Cabrera, M.; Šponer, J. E., "Theoretical Modeling on the Kinetics of the Arsenate-Ester Hydrolysis: Implications to the Stability of As-DNA", *Phys. Chem. Chem. Phys.* **13** (23), 10869–10871 (2011).

Muthukumar, K.; Yu, J.; Xu, Y.; Gulians, V. V., "Propane Ammonoxidation Over the MoV0Te-Nb-O M1 Phase: Reactivity of Surface Cations in Hydrogen Abstraction Steps," *Top. Catal.* **54**, 605–613 (2011).

Shelton, W. A.; Apra, E.; Sumpter, B. G.; Saraiva-Souza, A.; Souza filho, A. G.; Del Nero, J.; Meunier, V., "Theory of Zwitterionic Molecular-Based Organic Magnets," *Chem. Phys. Lett.* **511**, 294–298 (2011).

Simpson, M. L.; Cummings, P. T., "Fluctuations and Correlations in Physical and Biological Nanosystems: The Tale Is in the Tails," *ACS Nano* **5** (4), 2425–2432 (2011).

Šponer, J. E.; Šponer, J.; Fuentes-Cabrera, M., "Prebiotic Routes to Nucleotides: A Quantum Chemical Insight into the Energetics of the Multistep Reaction Pathways," *Chem. Eur. J.* **17** (3), 847–854 (2011).

Strobel, T. A.; Ganesh, P.; Somayazulu, M.; Kent, P.R.C.; Hemley, R. J., "Novel Cooperative Interactions and Structural Ordering in H₂S-H₂," *Phys. Rev. Lett.* **107** (25), 255503 (2011).

Su, S. Q.; Maier, T. A., "Coexistence of Strong Nematic and Superconducting Correlations in a Two-Dimensional Hubbard Model," *Phys. Rev. B* **84** (22), 220506 (2011).

Sun, Z. Z.; Xiao, K.; Keum, J. K.; Yu, X.; Hong, K. L.; Browning, J.; Ivanov, I. N.; Chen, J. H.; Alonzo, J.; Li, D. W.; Sumpter, B. G.; Payzant, E. A.; Rouleau, C. M.; Geohegan, D. B., "PS-*b*-P3HT Copolymers as P3HT/PCBM Interfacial Compatibilizers for High Efficiency Photovoltaics," *Adv. Mater.* **23** (46), 5529–5535 (2011).

Vazquez-Mayagoitia, A.; Horton, S. R.; Sumpter, B. G.; Šponer, J.; Šponer, J. E.; Fuentes-Cabrera, M., "On the Stabilization of Ribose by Silicate Minerals," *Astrobiology* **11** (2), 115–121 (2011).

Wang, X. J.; Hong, K. L.; Baskaran, D.; Goswami, M.; Sumpter, B.; Mays, J., "Asymmetrical Self-Assembly From Fluorinated and Sulfonated Block Copolymers in Aqueous Media," *Soft Matter* **7** (18), 7960–7964 (2011).

Wu, C. Y.; Skelton, A. A.; Chen, M. J.; Vlcek, L.; Cummings, P. T., "Modeling the Interaction Between Integrin-Binding Peptide (RGD) and Rutile Surface: The Effect of Na⁺ on Peptide Adsorption," *J. Phys. Chem. C* **115** (45), 22375–22386 (2011).

Wu, P.; Huang, J. S.; Meunier, V.; Sumpter, B. G.; Qiao, R., "Complex Capacitance Scaling in Ionic Liquids-Filled Nanopores," *ACS Nano* **5** (11), 9044–9051 (2011).

Xu, L. J.; Xu, Y., "Effect of Pd Surface Structure on the Activation of Methyl acetate," *Catal. Today* **165** (1), 96–105 (2011).

Yoo, J. J.; Balakrishnam, K.; Huang, J. S.; Meunier, V.; Sumpter, B. G.; Srivastava, A.; Conway, M.; Reddy, A.L.M.; Yu, J.; Vajtai, R.; Ajayan, P. M., " Ultrathin Planar Graphene Supercapacitors," *Nano Lett.* **11** (6), 1423–1427 (2011).

Yu, X.; Xiao, K.; Chen, J. H.; Lavrik, N. V.; Hong, K. L.; Sumpter, B. G.; Geohegan, D. B., "High-Performance Field-Effect Transistors Based on Polystyrene-*b*-Poly(3-hexylthiophene) Diblock Copolymers," *ACS Nano* **5** (5), 3559–3567 (2011).

Zhang, C. L.; Wang, M.; Luo, H. Q.; Wang, M. Y.; Liu, M. S.; Zhao, J.; Abernathy, D. L.; Maier, T. A.; Marty, K.; Lumsden, M. D.; Chi, S. X.; Chang, S.; Rodriguez-Rivera, J. A.; Lynn, J. W.; Xiang, T.; Hu, J. P.; Dai, P., "Neutron Scattering Studies of Spin Excitations in Hole-Doped Ba_{0.67}K_{0.33}Fe₂As₂ Superconductor," *Sci. Rep.* **1**, 115 (2011).

Zhang, X.; Song, X. H.; Zhang, X.-G.; Zhang, D. L., "Grain Boundary Resistivities of Polycrystalline Au Films," *Europhys. Lett.* **96** (1), 17010 (2011).

Zhang, Y.; Ke, X. Z.; Chen, C. F.; Yang, J. H.; Kent, P.R.C., "Nanodopant-Induced Band Modulation in AgPb_mSbTe_{2+m}-Type Thermoelectrics," *Phys. Rev. Lett.* **106** (20), 206601 (2011).

Zhang, Y.; Ke, X.; Kent, P.R.C.; Yang, J.; Chen, C., "Anomalous Lattice Dynamics Near the Ferroelectric Instability in PbTe," *Phys. Rev. Lett.* **107** (17), 175503 (2011).

Zhao, X. C., "Self-Assembly of DNA Segments on Graphene and Carbon Nanotube Arrays in Aqueous Solution: A Molecular Simulation Study," *J. Phys. Chem. C* **115** (14), 6181–6189 (2011).

Bajdich, M.; Reboreda, F. A.; Kent, P.R.C., "Quantum Monte Carlo Calculations of Dihydrogen Binding Energies on Ca Cations: An Assessment of Errors in Density Functionals for Weakly Bonded Systems," *Phys. Rev. B* **82** (8), 081405 (2010).

Bajdich, M.; Tiago, M. L.; Hood, R. Q.; Kent, P.R.C.; Reboreda, F. A., "Systematic Reduction of Sign Errors in Many-Body Calculations of Atoms and Molecules," *Phys. Rev. Lett.* **104**, 193001 (2010).

Clearfield, R.; Railsback, J. G.; Pearce, R. C.; Hensley, D. K.; Fowlkes, J. D.; Fuentes-Cabrera, M.; Simpson, M. L.; Rack, P. D.; Melechko, A. V., "Reactive Solid-State Dewetting of Cu-Ni Films on Silicon," *Appl. Phys. Lett.* **97** (25), 253101 (2010).

Cruz-Silva, E.; Botello-Mendez, A. R.; Barnett, Z. M.; Jia, M.; Dresselhaus, M. S.; Terrones, H.; Terrones, M.; Sumpter, B. G.; Meunier, V., "Controlling Edge Morphology in Graphene Layers Using Electron Irradiation: From Sharp Atomic Edges to Coalesced Layers Forming Loops," *Phys. Rev. Lett.* **105**, 045501 (2010).

Du, G. X.; Wang, S. G.; Ma, Q. L.; Wang, Y.; Ward, R.C.C.; Zhang, X.-G.; Wang, C.; Kohn, A.; Han, X. F., "Spin-Dependent Tunneling Spectroscopy for Interface Characterization of Epitaxial Fe/MgO/Fe Magnetic Tunnel Junctions," *Phys. Rev. B* **81**, 064438 (2010).

Feng, G.; Qiao, R.; Huang, J.; Sumpter, B. G.; Meunier, V., "Atomistic Insight on the Charging Energetics in Subnanometer Pore Supercapacitors," *J. Phys. Chem. C* **114**, 18012–18016 (2010).

Ford, D. C.; Nilekar, A. U.; Xu, Y.; Mavrikakis, M., "Partial and Complete Reduction of O₂ by Hydrogen on Transition Metal Surfaces," *Surf. Sci.* **604** (19–20), 1565–1575 (2010).

Goswami, M.; Sumpter, B. G.; Huang, T. Z.; Messman, J. M.; Gido, S. P.; Isaacs-Sodeye, A. I.; Mays, J. W., "Tunable Morphologies from Charged Block Copolymers," *Soft Matter* **6** (24), 6146–6154 (2010).

Goswami, M.; Sumpter, B. J.; Mays, J., "Controllable Stacked Disk Morphologies of Charged Diblock Copolymers," *Chem. Phys. Lett.* **487**, 272–278 (2010).

Govindasamy, A.; Muthukumar, K.; Yu, J.; Xu, Y.; Gulians, V. V., "Adsorption of Propane, Isopropyl, and Hydrogen on Cluster Models of the M1 Phase of Mo-V-Te-Nb-O Mixed Metal Oxide Catalyst," *J. Phys. Chem. C* **114** (10), 4544–4549 (2010).

Graser, S.; Kemper, A. F.; Maier, T. A.; Hirschfeld, P. J.; Scalapino, D. J., "Spin Fluctuations and Superconductivity in a Three-Dimensional Tight Binding Model for BaFe₂As₂," *Phys. Rev. B* **81** (21), 214503 (2010).

Huang, J. S.; Sumpter, B. G.; Meunier, V.; Yushin, G.; Portet, C.; Gogotsi, Y., "Curvature Effects in Carbon Nanomaterials: Exohedral Versus Endohedral Supercapacitors," *J. Mater. Res.* **25** (8), 1525–1531 (2010).

Huang, J. S.; Qiao, R.; Sumpter, B. G.; Meunier, V., "Effect of Diffuse Layer and Pore Shapes in Mesoporous Carbon Supercapacitors," *J. Mater. Res.* **25** (8), 1469–1475 (2010).

Kemper, A. F.; Maier, T. A.; Graser, S.; Cheng, H. P.; Hirschfeld, P. J.; Scalapino, D. J., "Sensitivity of the Superconducting State and Magnetic Susceptibility to Key Aspects of Electronic Structure in Ferropnictides," *New J. Phys.* **12**, 073030 (2010).

Lipton-Duffin, J. A.; Miwa, J. A.; Kondratenko, M.; Ciciora, F.; Sumpter, B. G.; Meunier, V.; Perepichka, D. F.; Rosei, F., "Step-by-Step Growth of Epitaxially Aligned Polythiophene by Surface-Confined Reaction," *Proc. Nat. Acad. Sci.* **107** (25), 11200–11204 (2010).

Maier, T. A.; Alvarez, G.; Summers, M.; Schulthess, T. C., "Dynamic Cluster Quantum Monte Carlo Simulations of a Two-Dimensional Hubbard Model with Stripelike Charge-Density-Wave Modulations: Interplay between Inhomogeneities and the Superconducting State," *Phys. Rev. Lett.* **104** (24), 247001 (2010).

Manjon, F. J.; Gomis, O.; Rodriguez-Hernandez, P.; Perez-Gonzalez, E.; Munoz, A.; Errandonea, D.; Ruiz-Fuertes, J.; Segura, A.; Fuentes-Cabrera, M.; Tiginyanu, I. M.; Uraski, V. V., "Nonlinear Pressure Dependence of the Direct Band Gap in Adamantine Ordered-Vacancy Compounds," *Phys. Rev. B* **81** (9), 195201 (2010).

Merkulov, I. A.; Alvarez, G.; Yakovlev, D. R.; Schultheiss, T. C., "Long-Term Dynamics of the Electron-Nuclear Spin System of a Semiconductor Quantum Dot," *Phys. Rev. B* **81** (11), 115107 (2010).

Meunier, V.; Pan, M. H.; Moreau, F.; Park, K. T.; Plummer, E. W., "Evidence of Coulomb Blockade Behavior in a Quasi-Zero-Dimensional Quantum Well on TiO₂ Surface," *Proc. Nat. Acad. Sci.* **107** (34), 14968–17972 (2010).

Okamoto, S.; Maier, T. A., "Microscopic Inhomogeneity and Superconducting Properties of a Two-Dimensional Hubbard Model for High-*T_c* Cuprates," *Phys. Rev. B* **81** (21), 214525 (2010).

Olcay, H.; Xu, L. J.; Xu, Y.; Huber, G. W., "Aqueous-Phase Hydrogenation of Acetic Acid over Transition Metal Catalysts," *ChemCatChem* **2** (11), 1420–1424 (2010).

Palma, J. L.; Cao, C.; Zhang, X.-G.; Krstic', P. S.; Krause, J. L.; Cheng, H.-P., "Manipulating I-V Characteristics of a Molecular Switch with Chemical Modifications," *J. Phys. Chem. C* **114**, 1655–1662 (2010).

Saha, K. K.; Lu, W. C.; Bernholc, J.; Meunier, V., "Electron Transport in Multiterminal Molecular Devices: A Density Functional Theory Study," *Phys. Rev. B* **81** (12), 125420 (2010).

Sen, C.; Alvarez, G.; Dagotto, E., "First Order Colossal Magnetoresistance Transitions in the Two-Orbital Model for Manganites," *Phys. Rev. Lett.* **105** (9), 097203 (2010).

Shin, J.; Borisevich, A. Y.; Meunier, V.; Zhou, J.; Plummer, E. W.; Kalinin, S. V.; Baddorf, A. P., "Oxygen-Induced Surface Reconstruction of SrRuO₃ and its Effect on the BaTiO₃ Interface," *ACS Nano* **4** (7), 4190–4196 (2010).

Šponer, J. E.; Vázquez-Mayagoitia, A.; Sumpter, B. G.; Leszczynski, J.; Šponer, J.; Otyepka, M.; Banáš, P.; Fuentes-Cabrera, M., "Theoretical Studies on the Intermolecular Interactions of Potentially Primordial Base-Pair Analogues," *Chem. Eur. J.* **16**, 3057–3065 (2010).

Sun, Y.; Burton, J. D.; Tsymbal, E. Y.; Electrically Driven Magnetism on a Pd Thin Film," *Phys. Rev. B* **81**, 064413 (2010).

Tselev, A.; Meunier, V.; Strelcov, E.; Shelton, W. A.; Luk'yanchuk, I. A.; Jones, K.; Proksch, R.; Kolmakov, A.; Kalinin, S. V., "Mesoscopic Metal-Insulator Transition at Ferroelastic Domain Walls in VO₂," *ACS Nano* **4** (8), 4412 (2010).

Vazquez-Mayagiotia, A.; Sherrill, C. D.; Apr, E.; Sumpter, B. G., "An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations," *J. Chem. Theory Comput.* **6** (3), 727–734 (2010).

Wang, W. X.; Wang, Y. P.; Zhang, X. -G.; Wang, Y.; Zou, J.; Han, X. F., "Thickness Dependence of Magnetic and Transport Properties in Organic-CoFe Discontinuous Multilayers," *J. Appl. Phys.* **107** (9), 09E307 (2010).

Wang, Y.; Zhang, J.; Zhang, X.-G.; Cheng, H. P.; Han, X. F., "First-Principles Study of Fe/MgO Based Magnetic Tunnel Junctions with Mg Interlayers," *Phys. Rev. B* **82** (5), 054405 (2010).

Wei, H. X.; Qin, Q. H.; Ma, G. L.; Zhang, X.-G.; Han, X. F., "Inelastic ElectronTunneling Spectrum From Surface Magnon and Magnetic Impurity Scatterings in Magnetic Tunnel Junctions," *Phys. Rev. B* **82** (13), 134436 (2010).

Xavier, J. C.; Alvarez, G.; Moreno, A.; Dagotto, E., "Coexistence of Pairing Tendencies and Ferromagnetism in a Doped Two-Orbital Hubbard Model on Two-Leg Ladders," *Phys. Rev. B* **81**, 085106 (2010).

Xiong, R. C.; Odbadrakh, K.; Michalkova, A.; Luna, J. P.; Petrova, T.; Keffer, D. J.; Nicholson, D. M.; Fuentes-Cabrera, M. A.; Lewis, J. P.; Leszczynski, J., "Evaluation of Functionalized Isoreticular Metal Organic Frameworks (IRMOFs) as Smart Nanoporous Preconcentrators of RDX," *Sens. Actuators, B* **148** (2), 459–468 (2010).

Xiong, R.; Keffer, D. J.; Fuentes-Cabrera, M.; Nicholson, D. M.; Michalkova, A.; Petrova, T.; Leszczynski, J.; Odbadrakh, K.; Doss, B. L.; Lewis, J. P., "Effect of Charge Distribution on RDX Adsorption in IRMOF-10," *Langmuir* **26** (8), 5942–5950 (2010).

Xu, L.; Xu, Y., "Activation of Methyl Acetate on Pd(111)," *Surf. Sci.* **604**, 887–892 (2010).

Zhang, J.; Wang, Y.; Zhang, X. -G.; Han, X. F., "Inverse and Oscillatory Magnetoresistance in Fe(001)/MgO/Cr/Fe Magnetic Tunnel Junctions," *Phys. Rev. B* **82** (13), 134449 (2010).

Zhang, X. -G.; Wen, Z. C.; Wei, H. X.; Han, X. F., "Giant Coulomb Blockade Magnetoresistance in Magnetic Tunnel Junctions with a Granular Layer," *Phys. Rev. B* **81** (15), 155122 (2010).

Bailey, C.; Fodor-Csorba, K.; Verduzco, R.; Gleeson, J. T.; Sprunt, S.; Jakli, A., "Large Flow Birefringence of Nemotogenic Bent-Core Liquid Crystals," *Phys. Rev. Lett.* **103** (23), 237803 (2009).

Botello-Méndez, A. R.; Cruz-Silva, E.; López-Urías, F.; Sumpter, B. G.; Meunier, V.; Terrones, M.; Terrones, H., "Spin Polarized Conductance in Hybrid Graphene Nanoribbons Using 5–7 Defects," *ACS Nano* **3** (11), 3606–3612 (2009).

Burton, J. D.; Tsymbal, E. Y.; "Prediction of Electrically Induced Magnetic Reconstruction at the Manganite/Ferroelectric Interface," *Phys. Rev. B* **80**, 174406 (2009).

Eisenbach, M.; Zhou, C.-G.; Nicholson, D. M.; Brown, D.; Larkin, J.; Schulhess, T. C., "A Scalable Method for *ab initio* Computation of Free Energies in Nanoscale Systems," *Proceedings of the Conference on High Performance Computing Networking, Storage and Analysis*, SC '09 November 14-20, 2009, Portland, Oregon, ACM (2009).

Iancu, V.; Kent, P.R.C.; Zeng, C. G.; Weitering, H. H., "Structure of YSi_2 Nanowires from Scanning Tunneling Spectroscopy and First-Principles," *Appl. Phys. Lett.* **95**, 123107 (2009).

Ke, X.; Chen, C.; Yang, J.; Wu, L.; Zhou, J.; Zhu, Y.; Kent, P.R.C., "Microstructure and a Nucleation Mechanism for Nanoprecipitates in $\text{PbTe}-\text{AgSbTe}_2$," *Phys. Rev. Lett.* **103**, 145502 (2009).

Kim, H.-Y.; Kent, P.R.C., "van der Waals Forces: Accurate Calculation and Assessment of Approximate Methods in Dielectric Nanocolloids up to 16 nm," *J. Chem. Phys.* **131**, 144705 (2009).

Li, J.; Jayaseker, T.; Meunier, V.; Mintmire, J. W., "Electronic Transport of Silicon Nanowires with Surface Defects," *Int. J. Quantum Chem.* **109**, 3705–3710 (2009).

Li, Y.; Lampkins, A. J.; Baker, M. B.; Sumpter, B. G.; Huang, J.; Abboud, K. A.; Castellano, R. K., "Benzotrifuanone: Synthesis, Structure, and Access to Polycyclic Heteroaromatics," *Org. Lett.* **11** (19), 4314–4317 (2009).

Muramatsu, H.; Hayashi, T.; Kim, Y. A.; Shimamoto, D.; Endo, M.; Meunier, V.; Sumpter, B. G.; Terrones, M.; Dresselhaus, M. S., "Bright Photoluminescence from the Inner Tubes of "Peapod"-Derived Double-Walled Carbon Nanotubes," *Small* **5** (23), 2678–2683 (2009).

Park, K. T.; Meunier, V.; Pan, M. H.; Shelton, W. A.; Yu, N.-H.; Plummer, E. W., "Nanoclusters of TiO_2 Wetted with Gold," *Surf. Sci.* **603**, 3131–3135 (2009).

Saha, K. K.; Lu, W.; Bernholc, J.; Meunier, V.; "First-Principles Methodology for Quantum Transport in Multiterminal Junctions," *J. Chem. Phys.* **131**, 164105 (2009).

Salafranca, J.; Alvarez, G.; Dagotto, E., "Electron-Lattice Coupling and Partial Nesting as the Origin of Fermi Arcs in Manganites," *Phys. Rev. B* **80** (15), 155133 (2009).

Sherrill, C. D.; Sumpter, B. G.; Sinnokrot, M. O.; Marshall, M. S.; Hohenstein, E. G.; Walker, R. C.; Gould, I. R., "Assessment of Standard Force Field Models Against High-Quality *Ab Initio* Potential Curves for Prototypes of $\pi-\pi$, CH/π , and SH/π Interactions," *J. Comput. Chem.* **30** (14), 2187–2198 (2009).

Vazquez-Mayagiotia, A.; Huertas, O.; Brancolini, G.; Migliore, A.; Sumpter, B. G.; Orozco, M.; Luque, F.J.; Di Felice, R.; Fuentes-Cabrera, M., "Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine," *J. Phys. Chem. B* **113**, 14465–14472 (2009).

Zhang, X. -G.; Pantelides, S. T., "Screening in Nanowires and Nanocontacts: Field Emission, Adhesion Force, and Contact Resistance," *Nano Lett.* **9** (12), 4306–4310 (2009).