Curriculum Vitæ: Qi An

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Education

Ph.D. Materials Science, California Institute of Technology, Pasadena, 2012.
M.S. Materials Science, California Institute of Technology, Pasadena, 2009.
M.S. Geophysics, University of Science and Technology of China, Hefei, 2007.
B.S. Geophysics, University of Science and Technology of China, Hefei, 2002.

Research Experience

Aug 2022–Now	**Associate Professor** AI-based Computational Materials Science; Computational Materials Design, Iowa State University.
Jul 2016–Jul 2022	**Assistant Professor** AI-based Computational Materials Science; Advanced Materials Design, University of Nevada, Reno.
Sep 2013–Jul 2016	**Research Scientist** Materials and Process Simulation Center, California Institute of Technology.
Jul 2012–Sep 2013	**Postdoctoral Scholar** Materials and Process Simulation Center, California Institute of Technology.
Summer 2008, 2010	**Graduate Internship** Theoretical Division, Los Alamos National Laboratory.

Research

- **Interest:** Quantum Mechanical Data-based Computational Materials Science: machine learning, machine learning force field, molecular dynamics simulations, quantum mechanics simulations, reactive force field and development. Some specific subject areas include:
  - Reinforcement learning: Determining complex activation processes in materials from zero knowledge.
  - Mechanical deformation and failure mechanism of semiconductors and superhard ceramics; photomechanical effects; stragetry to improve the mechanical properties of materials, and microstructural effects.
  - Mechanical properties of metal alloys and alloy design.

  - Deformation and damage of metals, and polymers under extreme loading conditions, and microstructural effects.
  - Haber-Bosch (HB) process: Reaction mechanism and kinetics on Fe surface; catalyst design to drastic improve the the reaction rates of HB process.
  - Bulk metallic glasses: forming ability, cavitation, and structural characterization.
  - Molten Salts: thermophysical properties.
  - Radiation damage; glass densification.
  - Detonation and sensitivity of energetic materials.
  - Thin film growth: diamond and gallium nitride thin film growth.
  - Phase transitions and kinetics, e.g., melting and crystallization.
  - Extended solid: structure prediction and property characterization.

- **Publication statistics**: about **180 journal papers** including 12 in *Physical Review Letters*, 4 in *Proceedings of the National Academy of Sciences*, 5 in *Journal of the American Chemical Society*, 1 in **Nature**, 1 in **Science**; ISI citations: 5064; **h-index: 39**.

Research Grants

- NSF-CMMI-2019459: Proposal Title: Collaborative Research: Photomechanical Behavior in Photovoltaic Semiconductors.
- NSF-CMMI-1727428: Proposal Title: Modeling and Design of Enhanced Strength and Ductility Through Grain Boundary Engineering–A Study of Boron Carbide Based Superhard Materials.
- ACS Petroleum Research Fund (PRF No. 58754-DNI6): Proposal Title: First Principles Multiscale Reactive Dynamics Modeling and Simulations to Predict Decomposition and Combustion of Clathrate Hydrates.
- DOE-NEUP: Proposal Title: Understanding the Speciation and Molecular Structure of Molten Salts Using In Situ Experimental Techniques and Atomistic Modeling.
- NSF-CMMI-2032483: Proposal Title: Understanding Dislocation Motion and Plasticity via First Principles Simulations Towards Manufacturing of High Ductility Magnesium Alloys.
- NSF-SBIR (subcontract from G-Space INC): Proposal Title: The Role of Gravity in Advanced Materials Manufacturing for the Era of Digital Transformation.

Awards

- Ralph E. Powe Junior Faculty Enhancement Award, OARU, 2018
- Liming Scholarship, California Institute of Technology, Pasadena, US, 2011.
- DongGang Scholarship, University of Science and Technology of China, Hefei, China, 2006.

- USTC outstanding Student Award, 2 times, University of Science and Technology of China, Hefei, China, 1997-2002.
- Zhang ZongZhi Scholarship, University of Science and Technology of China, Hefei, China, 2000.

Teaching Experience

- **Teaching Courses at University of Nevada Reno:**
  - **MSE 425/625** Introduction to Computational Materials Science
  - **MSE 433/633** Electronic, Magnetic and Optical Properties of Materials
  - **MSE 465/665** Nuclear Power Fundamentals
  - **MSE 468/668** Nuclear Materials
  - **MSE 472/672** Introduction to Ceramics
  - **MSE 742** Electronic Structure Theory and Applications
  - **MSE 791** The Physics Basis for Material Properties
- **Mentoring Graduate Students and Postdoctoral Scholars:**

  Dezhou Guo, PhD student, 2017 - 2020, post doc at Washington State University 2020 - .

  Topic: Atomistic simulations on detonation of energetic materials, reactions in clathrate, and failure mechanism of superhard ceramics.

  Joint papers: Phys. Rev. Lett. (2018), J. Phys. Chem. C (2018, 2020), ACS Appl. Mater. Interfaces (2018), Int. J. Plast. (2019), RSC Advances (2020).

  Yidi Shen, PhD student, 2017 - .

  Topic: Quantum mechanics and ReaxFF simulations on mechanical properites of Mg alloys, other metal alloys, and ceramics.

  Awards: Graduate Dean's Merit Scholarship of UNR, 2020; Doctoral Research in Innovation, Vision and Excellence Fellowship of UNR, 2021.

  Joint papers: J. Am. Ceram. Soc. (2018, 2021), Phys. Rev. B (2018), Scripta Mater. (2019), Phys. Rev. Mater. (2019), ACS Appl. Electron. Mater. (2019), J. Appl. Phys. (2019, 2021), JOM (2020).

  Fuller Jon, PhD student, 2018 - .

  Topic: Quantum mechanics simulations on molten salt structure and heterogeneous catalysis.

  Joint papers: Phys. Chem. Chem. Phys. (2019), Matter (2020), Chem. Mater. (2020).

  Jing Zhang, PhD student, 2018 - 2021.

  Topic: Quantum mechanics and machine learning force feild simulations on structure properties of Ti-alloys and molten salt, as well as corrosion mechnism of Zr-alloys.

  Joint papers: J. Phys. Chem. C (2020), J. Phys. Chem. B (2021).

Hongwei Wang, Post doc, 2018 - 2019, post doc at University of Minnesota 2019.

Topic: Advanced quantum mechanics simulations on photomechanical behavior of semiconductors

Joint papers: Phys. Rev. B (2019), J. Phys. Chem. C (2019), Phys. Chem. Chem. Phys. (2020).

Xiaokun Yang, Research staff, 2016 - 2017, post doc at Los Alamos National Lab 2017, since 2021 Staff scientist at Los Alamos National Lab.

Topic: Quantum mechanics simulations on structure and interficial properties of superhard ceramics

Joint papers: Phys. Chem. Chem. Phys. (2018), J. Phys. Chem. C (2018), ACS Appl. Mater. Interfaces (2018).

- **Other:**

  Participation in ACUE effective teaching training; received the *Certificatation in Effective College Instruction* on April 2020.

Synergistic Activities

- **Referee Experience**
  - **Scientific Journals:** *Journal of the American Chemical Society, Physical Review Letters, Nature Communications, Science Advances, ACS Nano, Nano Letters, Physical Review B, Acta Materialia, Scripta Materialia, The Journal of Physical Chemistry, The Journal of Chemical Physics, Journal of Applied Physics, and etc.*
  - **Research Grants:** *NSF (Regular and Career), DOE, and ARO* .
- **Editorial Board**: *Materials* (MDPI).
- **Member of Society**: SES, TMS, MRS, ACerS.
- **Symposium Organizer**: *Phase Transformations and Microstructural Evolution* (TMS meeting, 2021).
- **Session Chair**: General Topic I of *Phase Transformations and Microstructural Evolution* (TMS meeting, 2021).

Journal Publications (+: equal contribution; ∗: corresponding authorship)

177. M. Huang, P. Zhai, G.D. Li, **Q. An**, S.I. Morozov, W. Li, Q.Zhang, and W.A. Goddard III, Nanotwin-Induced Ductile Mechanism in Thermoelectric Semiconductor PbTe, *Matter*, 5, 1839–1852, 2022

176. Y. He, Y.D. Shen, B. Tang, and **Q. An***, ElectronHole Excitation Induced Softening in Boron Carbide-Based Superhard Materials, *ACS Applied Materials and Interfaces*, 14, 25792–25801, 2022

175. H. Wang, F. Tang, M. Stengel, H. Xiang, **Q. An***, T. Low, and X. Wu, Convert Widespread Paraelectric Perovskite to Ferroelectrics, *Physical Review Letters*, 128, 197601, 2022

174. X. Huang, Y.D. Shen, and **Q. An***, Nanotwinning Induced Decreased Lattice Thermal Conductivity of High Temperature Thermoelectric Boron Subphosphide (B12P2) from Deep Learning Potential Simulations, *Energy and AI*, 8, 100135, 2022

173. R. Karre, Y.D. Shen, S. Song, Y. Hu, S. Lahkar, X. Wang, **Q. An**, and K.M. Reddy, Shear Band Formation during Nanoindentation of EuB6 Rare-Earth Hexaboride, *Communications Materials*, 3, 1–9, 2022

172. Y.D. Shen, W.L. Johnson, K. Samwer, S.L. Corona, W.A. Goddard III, and **Q. An***, Shear Banding in Binary Cu-Zr Metallic Glass: Comparison of the G-Phase with L-Phase, *Frontiers in Materials*, 9, 886788, 2022

171. J. Fuller, **Q. An***, A. Fortunelli, and W.A. Goddard III, Reaction Mechanisms, Kinetics, and Improved Catalysts for Ammonia Synthesis from Hierarchical High Throughput Catalyst Design, *Accounts of Chemical Research*, 55, 1124–1134, 2022

170. J. Li, **Q. An***, and L. Liu A Strong Two-Dimensional Semiconductor l-B4C with High Carrier Mobility, *The Journal of Physical Chemistry C*, 126, 6036–6046, 2022

169. J. Fuller, W. Phillips, **Q. An***, and R. Gakhar. Coordination and Thermophysical Properties of Select Trivalent Lanthanides in LiCl-KCl, *Materials*, 15, 1478, 2022

168. J. Fuller, J. Moon, J. Zhang, D. Chidambaram, and **Q. An***. Coordination and Thermophysical Properties of Select Trivalent Lanthanides in LiCl-KCl, *Physical Chemistry Chemical Physics*, 24, 13102–13109, 2022

167. **Q. An***, W.L. Johnson, K. Samwer, S.L. Corona, Y.D. Shen, and W.A. Goddard III, The L-G Phase Transition in Binary Cu-Zr Metallic Liquids, *Physical Chemistry Chemical Physics*, 24, 497–506, 2022

166. J. Fuller, A. Fortunelli, W.A. Goddard III, and **Q. An***, Vibrational Spectroscopy Signatures of Catalytically Relevant Configurations for N2 Reduction to NH3 on Fe Surfaces via Density Functional Theory, *The Journal of Physical Chemistry C*, 125, 27919–27930, 2021

165. X.N. Huang, Y.J. Hu, and **Q. An***, Locking of Screw Dislocations in Silicon due to Core Structure Transformation, *The Journal of Physical Chemistry C*, 125, 24710–24718, 2021

164. T. Lan, and **Q. An***, Discovering Catalytic Reaction Networks Using Deep Reinforcement Learning from First Principles, *Journal of the American Chemical Society*, 143, 16804–16812, 2021

163. J. Li, **Q. An***, and L. Liu, Local Amorphization in Boron Carbide at Finite Temperature; Strategies toward Improved Ductility, *Physical Review B*, 104, 134105, 2021

162. **Q. An***, Mitigating Amorphization in Superhard Boron Carbide by Microalloying Induced Stacking Faults Formation, *Physical Review Materials*, 5, 103602, 2021

161. C. Hwang, J. Du, Q. Yang, A.M. Celik, K. Christian, **Qi An**, M.C. Schaefer, K.Y. Xie, J.C. LaSalvia, K.J. Hemker, W.A. Goddard III, and R.A. Haber, Addressing Amorphization and Transgranular Fracture of B4C through Si Doping and TiB2 Microparticle Reinforcing, *Journal of the American Ceramic Society*, 105, 2959–2977, 2021

160. KT Ramesh, L. Graham-Brady, W.A. Goddard III, R.C. Hurley, M. Robbins, A.L. Tonge, A. Bhattacharjee, J.T. Clemmer, Q. Zeng, W. Li, Y.D. Shen, **Q. An**, and N. Mitra, Models for the Behavior of Boron Carbide in Extreme Dynamic Environments, *Journal of the American Ceramic Society*, 105, 3043–3061, 2021

159. J. Zhang, J. Fuller, and **Q. An***, Coordination and Thermophysical Properties of Transition Metal Chlorocomplexes in LiCl-KCl Eutectic, *The Journal of Physical Chemistry B*, 125, 8876–8887, 2021

158. S.Z. Chavoshi, P.S. Branicio, and **Q. An**, Transition between Hall-Petch and inverse Hall-Petch Behavior in Nanocrystalline Silicon Carbide, *Physical Review Materials*, 5, 073606, 2021

157. Z. Lu, B. Huang, G.D. Li, X. Zhang, **Q. An**, B. Duan, P.C. Zhai, Q.J. Zhang, and W.A. Goddard III, Shear Induced Deformation Twinning Evolution in Thermoelectric InSb, *npj Computational Materials*, 7, 1–9, 2021

156. Y.D. Shen, M.Y. Yang, W.A. Goddard III, and **Q. An***, Strengthening Boron Carbide by Doping Si into Grain Boundaries, *Journal of the American Ceramic Society*, 105, 2978–2989, 2021.

155. P. Zhao, Z. Fang, X. Zhang, J. Chen. Y.D. Shen, X. Zhang, **Q. An**, C. Yang, X. Gao, S. Zhang, B. Tang, Aliovalent Doping Engineering for A- and B-Sites with Multiple Regulatory Mechanisms: A Strategy to Improve Energy Storage Properties of Sr0.7Bi0.2TiO3-Based Lead-Free Relaxor Ferroelectric Ceramics, *ACS Applied Materials and Interfaces*, 13, 24833–24855, 2021

154. Y.D. Shen, J. Fuller, and **Q. An***, Mitigating the Formation of Amorphous Shear Band in Boron Carbide, *Journal of Applied Physics*, 129, 140902, 2021 (Selected as the Featured Article and reported in AIP Scilight)

153. K. Xiao, X. Lei, Y. Chen, **Q. An**, D. Hu, C. Wang, X. Wu, and C. Huang, Extraordinary Impact Resistance of Carbon Nanotube Film with Crosslinks under Micro-Ballistic Impact, *Carbon*, 175, 478–489, 2021

152. G.D. Li, **Q. An**, B. Duan, L. Borgsmiller, M. Malki, M. Agne, U. Aydemir, P.C. Zhai, Q.J. Zhang, S.I. Morozov, W.A. Goddard III, and J. Snyder, Fracture Toughness of Thermoelectric Materials, *Materials Science and Engineering: R: Reports*, 144, 100607, 2021

151. **Q. An***, W.L. Johnson, K. Samwer, S.L. Corona, and W.A. Goddard III, The First Order L-G Phase Transition in Liquid Ag and Ag-Cu Alloys is Driven by Deviatoric Strain, *Scripta Materialia*, 194, 113695, 2021

150. H. Zhang, Y.D. Shen, S. Lahkar, T. Fujita, K. Hemker, **Q. An***, and K.M. Reddy, Distorted Planar Defects Stabilize Tetragonal Boron, *Scripta Materialia*, 194, 113685, 2021

149. N. Wang, Y.D. Shen, **Q. An**, K.M. Reddy, M. Jin, R. Karre, and X.D. Wang, Microstructure Evolution and Mechanical Property of Cu-15Ni-8Sn-0.2 Nb Alloy during Aging Treatment, *Journal of Materials Science and Technology*, 86, 227–236, 2021

148. S.A. Lindley$^+$, **Q. An**$^+$, W.A. Goddard III, and J.K. Cooper, Spatiotemporal Temperature and Pressure in Thermoplasmonic Gold Nanosphere-Water Systems, *ACS Nano*, 15, 6276–6288, 2021

147. Y. He, Y.D. Shen, B. Tang, and **Q. An***, Electro-Mechanical Coupling in FCC Metal Rhodium from First-Principles Simulations, *Journal of Materials Research*, 36, 2662–2673, 2021

146. K.M. Reddy, D.Z. Guo, S.X. Song, C. Cheng, J. Han, X.D. Wang, **Q. An**, and M.W. Chen, Dislocation-Mediated Shear Amorphization in Boron Carbide, *Science Advances*, 7(8), eabc6714, 2021

145. **Q. An***, Drastic Modification of Lattice Thermal Conductivity in Thermoelectrics Induced by Electron-Hole Pairs, *ACS Applied Materials and Interfaces*, 13, 3911–3918, 2021

144. **Q. An***, M. Mcdonald, A. Fortunelli, and W.A. Goddard III, Controlling the Shapes of Nanoparticles by Dopant-Induced Enhancement of Chemisorption and Catalytic Activity: Application to Fe-Based Ammonia Synthesis, *ACS Nano*, 15, 1675–1684, 2021

143. R. Karre, D.Z. Guo, S.X. Song, Y. Hu, Y. Liu, Q. Guo, P. Liu, X.D. Wang, **Q. An***, and K.M. Reddy, Vacancy-Driven Shear Localization in Silicon Nitride, *Scripta Materialia*, 190, 163–167, 2021

142. J. Fuller, A. Fortunelli, W.A. Goddard III, and **Q. An***, Discovery of Dramatically Improved Ammonia Synthesis Catalysts through Hierarchical High-Throughput Catalyst Screening of the Fe (211) Surface, *Chemistry of Materials*, 32, 9914–9924, 2020

141. J. Zhang, Y.D. Shen, H.W. Wang, and **Q. An***, Bi-doped Zirconium Alloys with Enhanced Water Oxidation Resistance, *The Journal of Physical Chemistry C*, 124, 23116–13125, 2020

140. B. Li, Y.D. Shen, and **Q. An**, Structural Origin of Reversible Martensitic Transformation and Reversible Twinning in NiTi Shape Memory Alloy, *Acta Materialia*, 199, 240–252, 2020

139. X.D. Wang, Y.D. Shen, S.X. Song, P. Liu, **Q. An***, and K.M. Reddy, Atomic-Scale Understanding of the $\gamma/\alpha 2$ Interface in a TiAl Alloy, *Journal of Alloys and Compounds*, 846, 156381, 2020

138. A.M. Gaffney, **Q. An**, W.A. Goddard III, W. Diao, and M.V. Glazoff, Toward Concurrent Engineering of the M1-Based Catalytic Systems for Oxidative Dehydrogenation (ODH) of Alkanes, *Topics in Catalysis*, 63, 1667–1682, 2020

137. Y. He, Y.D. Shen, B. Tang, and **Q. An***, Enhanced Strength and Ductility of Superhard Boron Carbide through Injecting Electrons, *Journal of the European Ceramic Society*, 40, 4428–4435, 2020

136. **Q. An***, W.L. Johnson, K. Samwer, S.L. Corona, and W.A. Goddard III, Formation of Two Glass Phases in Binary Cu-Ag Liquid, *Acta Materialia*, 195, 274–281, 2020

135. J. Fuller, and **Q. An***, Room-Temperature Plastic Deformation in Diamond Nanopillars, *Matter*, 2, 1082–1084, 2020

134. Y.D. Shen, and **Q. An***, Modified Failure Mechanism of Silicon through Excess Electrons and Holes, *JOM*, 72, 3160–3169, 2020

133. D.Z. Guo, S.V. Zybin, W.A. Goddard III, and **Q. An***, Enhancing the Detonation Properties of Liquid Nitromethane by Adding Nitro-Rich Molecule Nitryl Cyanide, *The Journal of Physical Chemistry C*, 124, 9787–9794, 2020

132. **Q. An***, M. Mcdonald, A. Fortunelli, and W.A. Goddard III, Si-doped Fe Catalyst for Ammonia Synthesis at Dramatically Decreased Pressures and Temperatures, *Journal of the American Chemical Society*, 142, 8223–8232, 2020

131. S.M. Sun, **Q. An**, M. Watanabe, J Cheng, H.H. Kim, T. Akbay, A. Takagaki, and T. Ishihara, Highly Correlation of CO2 Reduction Selectivity and Surface Electron Accumulation: A Case Study of Au-MoS2 and Ag-MoS2 Catalyst, *Applied Catalysis B: Environmental*, 271, 118931, 2020

130. G.D. Li, **Q. An**, U. Aydemir, S.I. Morozov, B. Duan, P.C. Zhai, Q.J. Zhang, and W.A. Goddard III, Intrinsic Mechanical Behavior of MgAgSb Thermoelectric Material: An ab Initio Study, *Journal of Materiomics*, 6, 24–32, 2020

129. Y. He, Y.D. Shen, B. Tang, and **Q. An***, Strengthening Boron Carbide through Lithium Dopant, *Journal of the American Ceramic Society*, 103, 2012–2023, 2020

128. M. Huang, G.D. Li, **Q. An**, P.C. Zhai, and W.A. Goddard III, Structural Failure of Layered Thermoelectric $In_4Se_{3-\delta}$ Semiconductors is Dominated by Shear Slippage, *Acta Materialia*, 187, 84–90, 2020

127. **Q. An***, W.L. Johnson, K. Samwer, S.L. Corona, and W.A. Goddard III, First Order Phase Transition in Liquid Ag to the Heterogeneous G-Phase, *The Journal of Physical Chemistry Letters*, 11, 632–645, 2020

126. D.Z. Guo, H.W. Wang, Y.D. Shen, and **Q. An***, Thermal Decomposition and Diffusion of Methane in Clathrate Hydrates from Quantum Mechanics Simulations, *RSC Advances*, 10, 14753–14760, 2020

125. H.W. Wang, J. Fuller, P. Chen, S.I. Morozov, and **Q. An***, Characterizing Local Metallic Bonding Variation Induced by External Perturbation, *Physical Chemistry Chemical Physics*, 22, 2372–2378, 2020

124. Y.D. Shen, H.W. Wang, and **Q. An***, Modified Generalized Stacking Fault Energy Surface of II-VI Ionic Crystals from Excess Electrons and Holes, *ACS Applied Electronic Materials*, 2, 56–65, 2020

123. Y.D. Shen, H.W. Wang, and **Q. An***, Enhanced Ductility of III-V Covalent Semiconductors from Electrons and Holes, *Journal of Applied Physics*, 126, 195105, 2019

122. H.W. Wang, S.X. Song, X.S. Zuo, F.X. Wang, Z.F. Zhang, S.I. Morozov, X.D. Wang, K.M. Reddy, and **Q. An***, Photomechanical Effect Leading to Extraordinary Ductility in Covalent Semiconductors, *Physical Review B*, 100, 094110, 2019

121. K.M. Reddy, D.Z. Guo, S. Lahkar, C. Cheng, Y. Shinoda, **Q. An***, and X.D. Wang, Graphite Interface Mediated Grain-Boundary Sliding Leads to Enhanced Mechanical Properties of Nanocrystalline Silicon Carbide, *Materialia*, 7, 100394, 2019

120. J.H. Zhou, Y. Yang, Y. Yang, D.S. Kim, A. Yuan, X.Z. Tian, C. Ophus, F. Sun, A.K. Schmid, M. Nathanson, H. Heinz, **Q. An**, H. Zeng, P. Ercius, and J.W. Miao, Observing Crystal Nucleation in Four Dimensions Using Atomic Electron Tomography, *Nature*, 570, 500–503, 2019

119. T. Cheng, A. Jaramillo-Botero, **Q. An**, D.V. Ilyin, S. Naserifar, and W.A. Goddard III, First Principles-based Multiscale Atomistic Methods for Input into First Principles Nonequilibrium Transport across Interfaces, *Proceedings of the National Academy of Sciences USA*, 116, 18193–18201, 2019

118. M. Mcdonald, J. Fuller, A. Fortunelli, W.A. Goddard III, and **Q. An***, Highly Efficient Ni-Doped Iron Catalyst for Ammonia Synthesis from QM-Based Hierarchical High Throughput Catalyst Screening, *The Journal of Physical Chemistry C*, 123, 17375–17383, 2019

117. D.G. Guo, and **Q. An***, Transgranular Amorphous Shear Band Formation in Polycrystalline Boron Carbide, *International Journal of Plasticity*, 121, 218–226, 2019

116. Y.D. Shen, H.W. Wang, B. Li, and **Q. An***, First Principles High-Throughput Screening to Enhance the Ductility of Lightweight Magnesium Alloys, *Physical Review Materials*, 3, 053603, 2019

115. H.W. Wang, and **Q. An***, Band-Gap Engineering in High-Temperature Boron-Rich Icosahedral Compounds, *The Journal of Physical Chemistry C*, 123, 12505–12513, 2019

114. H.W. Wang, S.I. Morozov, W.A. Goddard III, and **Q. An***, Light Irradiation Induced Brittle-to-Ductile and Ductile-to-Brittle Transition in Inorganic Semiconductors, *Physical Review B*, 99, 161202, 2019

113. C.C. Ye, **Q. An**, W.Q. Zhang, and W.A. Goddard III, Initial decomposition of HMX energetic material from quantum molecular dynamics and the molecular structure transition of β-HMX to δ-HMX, *The Journal of Physical Chemistry C*, 123, 9231–9236, 2019

112. J. Fuller, A. Fortunelli, W.A. Goddard III, and **Q. An***, Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(211) Reconstructed Surface, *Physical Chemistry Chemical Physics*, 21, 11444–11454, 2019

111. Y.D. Shen, G.D. Li, and **Q. An***, Enhanced Fracture Toughness of Boron Carbide from Microalloying and Nanotwinning, *Scripta Materialia*, 162, 306–310, 2019

110. G.D. Li, J.G. He, **Q. An**, S.I. Morozov, S.Q. Hao, P.C. Zhai, Q.J. Zhang, W.A. Goddard III, and G.J. Snyder, Dramatically Reduced Lattice Thermal Conductivity of Mg2Si Thermoelectric Material from Nanotwinning, *Acta Materialia*, 169, 9–14, 2019

109. Y. Gao, Y.Z. Ma, **Q. An**, V. Levitas, Y. Zhang, B. Feng, J. Chaudhuri, and W.A. Goddard III, Shear Driven Formation of Nano-Diamonds at Sub-Gigapascals and 300 K, *Carbon*, 146, 364–368, 2019

108. B. Tang, Y. He, W.A. Goddard III, and **Q. An***, First Principles Predicting Enhanced Ductility of Boride Carbide through Magnesium Microalloying, *Journal of the American Ceramic Society*, 102, 5514–5523, 2019

107. K.M. Reddy, P. Liu, Y.D. Shen, T. Goto, **Q. An***, and M.W. Chen, Atomic Structure and Mechanical Response of Coincident Stacking Faults in Boron Suboxide, *Materials Research Letters*, 7, 75–81, 2019

106. D.Z. Guo, and **Q. An***, Thermal Stability and Detonation Properties of Potassium 4,4-Bis(dinitromethyl)-3,3-azofurazanate, an Environmentally Friendly Energetic Three-Dimensional Metal-Organic Framework, *ACS Applied Materials and Interfaces*, 11, 1512–1519, 2018

105. **Q. An***, Y.D. Shen, A. Fortunelli, and W.A. Goddard III, QM-Mechanism-Based Hierarchical High-Throughput in silico Screening Catalyst Design for Ammonia Synthesis, *Journal of the American Chemical Society*, 140, 17702–17710, 2018

104. Y.D. Shen, and **Q. An***, Brittle Failure of Orthorhombic Borides from First-Principles Simulations, *Physical Review B*, 98, 134105, 2018

103. D.Z. Guo, D. Guo, F. Huang, and **Q. An***, Influence of Silicon on the Detonation Performance of Energetic Materials from First-Principles Molecular Dynamics Simulations, *The Journal of Physical Chemistry C*, 122, 24481–24487, 2018

102. Z. Mei, **Q. An**, F.Q. Zhao, S.Y. Xu, and X.H. Ju, Reactive Molecular Dynamics Simulation of Thermal Decomposition for Nano-Aluminized Explosives, *Physical Chemistry Chemical Physics*, 20, 29341–29350, 2018

101. D.Z. Guo, S. Song, R. Luo, W.A. Goddard III, M.W. Chen, K.M. Reddy, and **Q. An***, Grain Boundary Sliding and Amorphization are Responsible for the Reverse Hall-Petch Relation in Superhard Nanocrystalline Boron Carbide, *Physical Review Letters*, 121, 145504, 2018

100. G.D. Li, **Q. An**, S.I. Morozov, B. Duan, W.A. Goddard III, P.C. Zhai,Q.J. Zhang, and G.J. Snyder, Mechanical Softening of Thermoelectric Semiconductor Mg2Si from Nanotwinning, *Scripta Materialia*, 157, 90–94, 2018

99. J.H. Luo, L.Y. Chen, D.N. Nguyer, D.Z. Guo, **Q. An***, and M.J. Cheng, Dual Functions of Water in Stabilizing Metal-Pentazolate Hydrates [M(N5)2(H2O)4]4H2O (M = Mn, Fe, Co, and Zn) High-Energy-Density Materials, *The Journal of Physical Chemistry C*, 122, 21192–21201, 2018

98. A.U. Khan, A.M. Etzold, X.K. Yang, V. Domnich, K.Y. Xie, C. Hwang, S.I. Behler, M.W. Chen, **Q. An**, J.C. LaSalvia, K.J. Hemker, W.A. Goddard III, and R.A. Haber, Locating Si Atoms in Si-doped Boron Carbide: A Route to Understand Amorphization Mitigation Mechanism, *Acta Materialia*, 157, 106–113, 2018

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19. Yidi Shen, and **Q. An**, Electron-Hole Carriers Induced Microstructure Evolution in Inorganic Semiconductors, 2021 TMS Annual Meeting and Exhibition; Virtual meeting, March 15–18 (2021).

18. **(INVITED) Q. An**, Haber-Bosch Reaction Mechanism and Kinetics on Highly Reactive Iron Surface and in Silico Catalyst Design for Improved Reaction Rate, Seminar at Chemical and Biomedical Engineering, Cleveland State University, Cleveland, OH, March 18 (2021).

17. **Q. An**, The Physics of an Elemental Ag Glass: First Order Glass Transition and Melting, 2020 TMS Annual Meeting and Exhibition, San Diego, California, February 23–27 (2020).

16. **Q. An**, Haber-Bosch Reaction Mechanism and Kinetics on Highly Reactive Iron Surface and Hierarchical High-throughput in Silico Screening Catalyst Design, 2020 TMS Annual Meeting and Exhibition, San Diego, California, February 23–27 (2020).

15. **(INVITED) Q. An**, Dislocation or Twinning Formation in Inorganic Semiconductors under Light Irradiation, International Conference on Plasticity, Damage, and Fracture; Barcelo Maya Grand Resort, Rivera Maya, Mxico, Jan. 3–7, 2020.

14. **Q. An**, QM based high-throughput screening to enhance the ductility of lightweight magnesium alloys"; International Conference on Plasticity, Damage, and Fracture, Barcelo Maya Grand Resort, Rivera Maya, Mxico, Jan. 3–7, 2020.

13. **Q. An**, Haber-Bosch Reaction Mechanism and Kinetics on Highly Reactive Iron Surface and Hierarchical High-Throughput In Silico Screening Catalyst Design, 2019 MRS Annual Meeting and Exhibition, Boston, MA, Dec. 1–4, (2019).

12. **Q. An**, Grain Boundary Engineering Leading to Enhanced Mechanical Properties of Superhard Boron Carbide, 2019 MRS Annual Meeting and Exhibition, Boston, MA, Dec. 1–4, (2019).

11. **Q. An**, First Principles High-Throughput Screening to Enhance the Ductility of Lightweight Magnesium Alloys, 2019 MRS Annual Meeting and Exhibition, Boston, MA, Dec. 1–4, (2019).

10. **(INVITED) Q. An**, Achieving Enhanced Mechanical Properties of B4C through Grain Boundaries Engineering, CMGR meeting, MEDE program, John Hopkins University, Baltimore, MD (July 14, 2019).

9. **Q. An**, The Physics of an Elemental Ag Glass: First Order Glass Transition and Melting, Workshop at Caltech to Celebrate William Johnson's 70th Birthday, June 19–21 (2019).

8. **Q. An**, Amorphous Shear Bands Formation in Superhard Boron Carbide and Strategies to Improve its Strength and Ductility, Workshop at Caltech to Celebrate William Goddard III's 83th Birthday, Mar. 28–30 (2019).

7. **(INVITED) Q. An**, Brittle Failure of Boron Carbide and Related Superhard Materials from Atomistic Simulations; Strategy to Improve Ductility, 25th International Conference on Plasticity, Damage and Fracture, Panama City, Panama, Jan. 3–9 (2019).

6. **Q. An**, Reaction Mechanisms and Kinetics of Ammonia Synthesis on Fe(111) Surface, 2018 MRS Annual Meeting and Exhibition, Boston, MA, Nov. 28, (2018).

5. **(INVITED) Q. An**, Materials Design from First Principles Based Atomistic Modeling and Simulations, Seminar at Department of Physics, University of Nevada, Las Vegas (Sept. 7, 2018).

4. **Q. An**, Improving the Ductility of Boron Carbide from Computational Design, 2018 TMS Annual Meeting and Exhibition, Phoenix Convention Center, Phoenix Mar. 11–15 (2018).

3. **(INVITED) Q. An**, Atomistic Mechanisms underlying Brittle Failure of Boron Carbide based Superhard Materials, The 26th International Conference on High Pressure Science and Technology (AIRAPT 26), Beijing, China, Aug. 23 (2017).

2. **Q. An**, Atomistic Mechanisms underlying Brittle Failure of Boron Carbide based Superhard Materials, Seminar at Army Research Lab, Aberdeen, Maryland, Apr. 12 (2017).

1. **(INVITED) Q. An**, Nanotwins in Boron Carbide and Related Materials, 41st International Conference and Exposition on Advanced Ceramics and Composites, Daytona Beach, FL, Jan. 24 (2017).