## Gyeong S Hwang

List of Publications by Year in descending order

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87888 69250 6,442 148 38 77 citations h-index g-index papers 152 152 152 9305 docs citations times ranked citing authors all docs

| #  | Article  | IF              | CITATIONS    |
|----|--|-----------------|--------------|
| 1  | Long-life Li/polysulphide batteries with high sulphur loading enabled by lightweight three-dimensional nitrogen/sulphur-codoped graphene sponge. Nature Communications, 2015, 6, 7760.   | 12.8            | 923          |
| 2  | Freestanding 1T MoS <sub>2</sub> /graphene heterostructures as a highly efficient electrocatalyst for lithium polysulfides in Li–S batteries. Energy and Environmental Science, 2019, 12, 344-350.   | 30.8            | 510          |
| 3  | Factors in the Metal Doping of BiVO <sub>4</sub> for Improved Photoelectrocatalytic Activity as Studied by Scanning Electrochemical Microscopy and First-Principles Density-Functional Calculation. Journal of Physical Chemistry C, 2011, 115, 17870-17879. | 3.1             | 409          |
| 4  | On the Origin of the Enhanced Supercapacitor Performance of Nitrogen-Doped Graphene. Journal of Physical Chemistry C, 2013, 117, 5610-5616.  | 3.1             | 230          |
| 5  | A Computational Study of the Interfacial Structure and Capacitance of Graphene in [BMIM][PF <sub>6</sub> ] Ionic Liquid. Journal of the Electrochemical Society, 2013, 160, A1-A10.  | 2.9             | 229          |
| 6  | Structure and Properties of Liâ^'Si Alloys: A First-Principles Study. Journal of Physical Chemistry C, 2011, 115, 2514-2521.   | 3.1             | 187          |
| 7  | Highâ€Performance Lithiumâ€Sulfur Batteries with a Selfâ€Supported, 3D Li <sub>2</sub> Sâ€Doped Graphene<br>Aerogel Cathodes. Advanced Energy Materials, 2016, 6, 1501355.   | 19.5            | 183          |
| 8  | Large Thermoelectric Figure-of-Merits from SiGe Nanowires by Simultaneously Measuring Electrical and Thermal Transport Properties. Nano Letters, 2012, 12, 2918-2923.  | 9.1             | 181          |
| 9  | Nanocolumnar Germanium Thin Films as a High-Rate Sodium-Ion Battery Anode Material. Journal of Physical Chemistry C, 2013, 117, 18885-18890.   | 3.1             | 175          |
| 10 | Epoxide reduction with hydrazine on graphene: A first principles study. Journal of Chemical Physics, 2009, 131, 064704.  | 3.0             | 151          |
| 11 | On the Role of Pd Ensembles in Selective H <sub>2</sub> O <sub>2</sub> Formation on PdAu Alloys. Journal of Physical Chemistry C, 2009, 113, 12943-12945.  | 3.1             | 125          |
| 12 | A Comparative First-Principles Study of the Structure, Energetics, and Properties of Li–M (M = Si, Ge,) Tj ETQq0   | 0.0 rgBT<br>3.1 | /Oyerlock 10 |
| 13 | A Comparative First-Principles Study on Sodiation of Silicon, Germanium, and Tin for Sodium-Ion Batteries. Journal of Physical Chemistry C, 2015, 119, 14843-14850.  | 3.1             | 95           |
| 14 | Reaction mechanisms of aqueous monoethanolamine with carbon dioxide: a combined quantum chemical and molecular dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 831-839.   | 2.8             | 95           |
| 15 | Adsorption of Au atoms on stoichiometric and reduced TiO2(110) rutile surfaces: a first principles study. Surface Science, 2003, 542, 72-80.   | 1.9             | 87           |
| 16 | On the Nature and Behavior of Li Atoms in Si: A First Principles Study. Journal of Physical Chemistry C, 2010, 114, 17942-17946.   | 3.1             | 82           |
| 17 | Electron small polarons and their transport in bismuth vanadate: a first principles study. Physical Chemistry Chemical Physics, 2015, 17, 256-260.   | 2.8             | 81           |
| 18 | Lithiation Behavior of Silicon-Rich Oxide (SiO <sub>1/3</sub> ): A First-Principles Study. Chemistry of Materials, 2013, 25, 3435-3440.  | 6.7             | 80           |

| #  | Article   | IF   | CITATIONS |
|----|---|------|-----------|
| 19 | Tailoring the performance of graphene-based supercapacitors using topological defects: A theoretical assessment. Carbon, 2014, 68, 734-741.   | 10.3 | 78        |
| 20 | Structural phase-dependent hole localization and transport in bismuth vanadate. Physical Review B, 2013, 87, .  | 3.2  | 71        |
| 21 | Fundamental Understanding of CO <sub>2</sub> Capture and Regeneration in Aqueous Amines from First-Principles Studies: Recent Progress and Remaining Challenges. Industrial & Engineering Chemistry Research, 2017, 56, 6887-6899.                    | 3.7  | 70        |
| 22 | Relative contributions of quantum and double layer capacitance to the supercapacitor performance of carbon nanotubes in an ionic liquid. Physical Chemistry Chemical Physics, 2013, 15, 19741-19747.  | 2.8  | 68        |
| 23 | Effects of vacancy defects on thermal conductivity in crystalline silicon: A nonequilibrium molecular dynamics study. Physical Review B, 2011, 83, .  | 3.2  | 65        |
| 24 | Growth and structure of small gold particles on rutileTiO2(110). Physical Review B, 2005, 72, .   | 3.2  | 62        |
| 25 | Dynamics of oxygen species on reducedTiO2(110)rutile. Physical Review B, 2004, 70, .  | 3.2  | 60        |
| 26 | Geometric Parameter Effects on Ensemble Contributions to Catalysis: H <sub>2</sub> O <sub>2</sub> Formation from H <sub>2</sub> and O <sub>2</sub> on AuPd Alloys. A First Principles Study. Journal of Physical Chemistry C, 2010, 114, 14922-14928. | 3.1  | 56        |
| 27 | Hybrid density functional study of the structural, bonding, and electronic properties of bismuth vanadate. Physical Review B, 2012, 86, .   | 3.2  | 55        |
| 28 | Impact of Graphene Edges on Enhancing the Performance of Electrochemical Double Layer Capacitors. Journal of Physical Chemistry C, 2014, 118, 21770-21777.  | 3.1  | 54        |
| 29 | Curvature Effects on the Interfacial Capacitance of Carbon Nanotubes in an Ionic Liquid. Journal of Physical Chemistry C, 2013, 117, 23539-23546.   | 3.1  | 53        |
| 30 | Magnetoâ€convection in a rotating layer of nanofluid. Asia-Pacific Journal of Chemical Engineering, 2014, 9, 663-677.   | 1.5  | 50        |
| 31 | The Bright Future for Electrode Materials of Energy Devices: Highly Conductive Porous Na-Embedded Carbon. Nano Letters, 2016, 16, 8029-8033.  | 9.1  | 50        |
| 32 | On the origin of the significant difference in lithiation behavior between silicon and germanium. Journal of Power Sources, 2014, 263, 252-258.   | 7.8  | 44        |
| 33 | On the influence of polarization effects in predicting the interfacial structure and capacitance of graphene-like electrodes in ionic liquids. Journal of Chemical Physics, 2015, 142, 024701.  | 3.0  | 44        |
| 34 | Toward a Reversible Calciumâ€Sulfur Battery with a Lithiumâ€Ion Mediation Approach. Advanced Energy Materials, 2019, 9, 1803794.  | 19.5 | 43        |
| 35 | On the origin of Si nanocrystal formation in a Si suboxide matrix. Journal of Applied Physics, 2007, 102,   | 2.5  | 41        |
| 36 | Role of Small Pd Ensembles in Boosting CO Oxidation in AuPd Alloys. Journal of Physical Chemistry Letters, 2012, 3, 566-570.  | 4.6  | 40        |

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|----|--|-----|-----------|
| 37 | Large Capacitance Enhancement Induced by Metal-Doping in Graphene-Based Supercapacitors: A First-Principles-Based Assessment. ACS Applied Materials & Interfaces, 2014, 6, 12168-12176.                                  | 8.0 | 40        |
| 38 | Diffusion and dissociation of neutral divacancies in crystalline silicon. Physical Review B, 2002, 65, .   | 3.2 | 39        |
| 39 | Structure and Li <sup>+</sup> ion transport in a mixed carbonate/LiPF <sub>6</sub> electrolyte near graphite electrode surfaces: a molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 27868-27876. | 2.8 | 39        |
| 40 | On the origin of preferred bicarbonate production from carbon dioxide (CO <sub>2</sub> ) capture in aqueous 2-amino-2-methyl-1-propanol (AMP). Physical Chemistry Chemical Physics, 2015, 17, 29184-29192.               | 2.8 | 38        |
| 41 | Force-matching-based parameterization of the Stillinger-Weber potential for thermal conduction in silicon. Physical Review B, 2012, 85, .  | 3.2 | 37        |
| 42 | Communication: Enhanced oxygen reduction reaction and its underlying mechanism in Pd-Ir-Co trimetallic alloys. Journal of Chemical Physics, 2013, 139, 201104.   | 3.0 | 37        |
| 43 | Charging Rate Dependence of Ion Migration and Stagnation in Ionic-Liquid-Filled Carbon Nanopores.<br>Journal of Physical Chemistry C, 2016, 120, 24560-24567.  | 3.1 | 35        |
| 44 | O2-coverage-dependent CO oxidation on reduced TiO2(110): A first principles study. Journal of Chemical Physics, 2006, 125, 144706.   | 3.0 | 34        |
| 45 | Structure and stability of small compact self-interstitial clusters in crystalline silicon. Physical Review B, 2008, 77, .   | 3.2 | 34        |
| 46 | Pd ensemble effects on oxygen hydrogenation in AuPd alloys: A combined density functional theory and Monte Carlo study. Catalysis Today, 2011, 165, 138-144.   | 4.4 | 34        |
| 47 | Structure of small Aun, Agn, and Cun clusters (n=2â^4) on rutile TiO2(110): A density functional theory study. Computational and Theoretical Chemistry, 2006, 771, 129-133.  | 1.5 | 31        |
| 48 | Mechanism of thermal conductivity suppression in doped silicon studied with nonequilibrium molecular dynamics. Physical Review B, 2012, 86, .  | 3.2 | 30        |
| 49 | A channel for dimer flipping on the Si(001) surface. Surface Science, 2000, 465, L789-L793.  | 1.9 | 27        |
| 50 | Structure, energetics, and bonding of amorphous Au–Si alloys. Journal of Chemical Physics, 2007, 127, 224710.  | 3.0 | 27        |
| 51 | Growth and shape transition of small silicon self-interstitial clusters. Physical Review B, 2008, 78, .  | 3.2 | 27        |
| 52 | Origin of nonlocal interactions in adsorption of polar molecules on Si(001)-2 $\tilde{A}$ -1. Journal of Chemical Physics, 2005, 122, 164706.  | 3.0 | 26        |
| 53 | Structure, stability, and diffusion of arsenic-silicon interstitial pairs. Applied Physics Letters, 2005, 87, 231905.  | 3.3 | 26        |
| 54 | First-principles assessment of CO <sub>2</sub> capture mechanisms in aqueous piperazine solution. Physical Chemistry Chemical Physics, 2016, 18, 25296-25307.  | 2.8 | 26        |

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|----|---|------|-----------|
| 55 | Silicon interstitials atSiâ <sup>*</sup> ·SiO2interfaces: Density functional calculations. Physical Review B, 2005, 72, .   | 3.2  | 24        |
| 56 | First-principles study of the mechanical and optical properties of amorphous hydrogenated silicon and silicon-rich silicon oxide. Physical Review B, 2010, 81, .  | 3.2  | 24        |
| 57 | Atomic Arrangements of AuPt/Pt(111) and AuPd/Pd(111) Surface Alloys: A Combined Density Functional Theory and Monte Carlo Study. Journal of Physical Chemistry C, 2010, 114, 21516-21523.   | 3.1  | 24        |
| 58 | Structure and Interconversion of Oxygen-Vacancy-Related Defects on Amorphous Silica. Physical Review Letters, 2006, 97, 066101.   | 7.8  | 23        |
| 59 | Theoretical Analysis of Thermal Transport in Graphene Supported on Hexagonal Boron Nitride: The Importance of Strong Adhesion Due to <mml:math display="inline" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï€</mml:mi></mml:math> -Bond Polarization. Physical Review Applied, 2016, 6, . | 3.8  | 23        |
| 60 | Nucleation and growth of 1B metal clusters on rutile TiO2(110): Atomic level understanding from first principles studies. Catalysis Today, 2005, $105$ , $78-84$ .  | 4.4  | 22        |
| 61 | Molecular mechanisms for thermal degradation of CO <sub>2</sub> -loaded aqueous monoethanolamine solution: a first-principles study. Physical Chemistry Chemical Physics, 2019, 21, 22132-22139.  | 2.8  | 22        |
| 62 | Interstitial-Mediated Arsenic Clustering in Ultrashallow Junction Formation. Electrochemical and Solid-State Letters, 2006, 9, G354.  | 2.2  | 21        |
| 63 | Strain-Induced Formation of Surface Defects in Amorphous Silica: A Theoretical Prediction. Physical Review Letters, 2008, 100, 076104.  | 7.8  | 21        |
| 64 | A comparative theoretical study of Au, Ag and Cu adsorption on TiO2 (110) rutile surfaces. Korean Journal of Chemical Engineering, 2004, 21, 537-547.   | 2.7  | 20        |
| 65 | Synergetic Role of Photogenerated Electrons and Holes in the Oxidation of CO to CO <sub>2</sub> on Reduced TiO <sub>2</sub> (110): A First-Principles Study. ACS Catalysis, 2014, 4, 4051-4056.   | 11.2 | 20        |
| 66 | Interaction of oxygen with polystyrene and polyethylene polymer films: A mechanistic study. Journal of Applied Physics, 2020, 127, .  | 2.5  | 20        |
| 67 | A computational analysis of graphene adhesion on amorphous silica. Journal of Applied Physics, 2013, 113, 164901.   | 2.5  | 19        |
| 68 | Molecular Insights into the Complex Relationship between Capacitance and Pore Morphology in Nanoporous Carbon-based Supercapacitors. ACS Applied Materials & Samp; Interfaces, 2016, 8, 34659-34667.  | 8.0  | 19        |
| 69 | Psesudocubic Phase Tungsten Oxide as a Photocatalyst for Hydrogen Evolution Reaction. ACS Applied Energy Materials, 2019, 2, 8792-8800.   | 5.1  | 19        |
| 70 | Theoretical determination of stable fourfold coordinated vacancy clusters in silicon. Physical Review B, 2008, 78, .  | 3.2  | 18        |
| 71 | What is the thermal conductivity limit of silicon germanium alloys?. Physical Chemistry Chemical Physics, 2016, 18, 19544-19548.  | 2.8  | 18        |
| 72 | Effects of P on amorphous chemical vapor deposition Ru-P alloy films for Cu interconnect liner applications. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2008, 26, 974-979.   | 2.1  | 17        |

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| 73 | On the Nature and Origin of Si Surface Segregation in Amorphous AuSi Alloys. Journal of Physical Chemistry C, 2010, 114, 3037-3041.  | 3.1         | 17          |
| 74 | Molecular insights into the enhanced rate of CO2 absorption to produce bicarbonate in aqueous 2-amino-2-methyl-1-propanol. Physical Chemistry Chemical Physics, 2017, 19, 32116-32124. | 2.8         | 16          |
| 75 | Controlling Plasmonâ€Enhanced Fluorescence via Intersystem Crossing in Photoswitchable Molecules. Small, 2017, 13, 1701763.  | 10.0        | 15          |
| 76 | Diffusion of the Diboron Pair in Silicon. Physical Review Letters, 2002, 89, 055901.   | 7.8         | 14          |
| 77 | On the origin of anisotropic lithiation in crystalline silicon over germanium: A first principles study. Applied Surface Science, 2014, 323, 78-81.                                    | 6.1         | 14          |
| 78 | Importance of Pd monomer pairs in enhancing the oxygen reduction reaction activity of the AuPd(1 0) Tj ETQq0   | 0 0 rgBT /0 | Overlock 10 |
| 79 | Partial oxidation of methane to methanol by isolated Pt catalyst supported on a CeO2 nanoparticle. Journal of Chemical Physics, 2020, 152, 054715.                                     | 3.0         | 14          |
| 80 | Interaction of neutral vacancies and interstitials with the Si (001) surface. Physical Review B, 2004, 70, .   | 3.2         | 13          |
| 81 | Interstitial-mediated mechanisms of As and P diffusion in Si: Gradient-corrected density-functional calculations. Physical Review B, 2006, 74.   | 3.2         | 13          |
| 82 | display="inline"> <mml:mrow><mml:msub><mml:mrow< td=""><td></td><td></td></mml:mrow<></mml:msub></mml:mrow>  |             |             |
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| 91  | Combined experimental and computational study on the promising monoethanolamineÂ+Â2-(ethylamino)ethanolÂ+Âsulfolane biphasic aqueous solution for CO2 absorption. Chemical Engineering Journal, 2022, 446, 136674.                                       | 12.7 | 11        |
| 92  | Atomistic structural description of the $Si(001)/\langle i\rangle a\langle i\rangle -SiO\langle sub\rangle 2\langle sub\rangle interface$ : The influence of different Keating-like potential parameters. Journal of Applied Physics, 2011, 109, 113519. | 2.5  | 10        |
| 93  | Anomalous Facile Carbamate Formation at High Stripping Temperatures from Carbon Dioxide Reaction with 2-Amino-2-methyl-1-propanol in Aqueous Solution. ACS Sustainable Chemistry and Engineering, 2020, 8, 18671-18677.                                  | 6.7  | 10        |
| 94  | Dissociative chemisorption of methyl fluoride and its implications for atomic layer etching of silicon nitride. Applied Surface Science, 2021, 543, 148557.  | 6.1  | 10        |
| 95  | An experimental/computational study of steric hindrance effects on <scp>CO<sub>2</sub></scp> absorption in (non)aqueous amine solutions. AICHE Journal, 2022, 68, .  | 3.6  | 10        |
| 96  | Shouldering in B diffusion profiles in Si: Role of di-boron diffusion. Applied Physics Letters, 2003, 83, 3501-3503.   | 3.3  | 9         |
| 97  | Surface chemistry effects on vacancy and interstitial annihilation on Si(001). Physica Status Solidi (B): Basic Research, 2004, 241, 2303-2312.  | 1.5  | 9         |
| 98  | Structure and dynamics of the diarsenic complex in crystalline silicon. Physical Review B, 2005, 72, .   | 3.2  | 9         |
| 99  | Biaxial strain effects on the structure and stability of self-interstitial clusters in silicon. Physical Review B, 2009, 79, .   | 3.2  | 9         |
| 100 | Atomic Arrangements in AuPt/Pt(100) and AuPd/Pd(100) Surface Alloys: A Monte Carlo Study Using First Principles-Based Cluster Expansions. Journal of Physical Chemistry C, 2011, 115, 21205-21210.   | 3.1  | 9         |
| 101 | Role of the surface–subsurface interlayer interaction in enhancing oxygen hydrogenation to water in Pd3Co alloy catalysts. Physical Chemistry Chemical Physics, 2013, 15, 12118.   | 2.8  | 9         |
| 102 | Anomalous Stagewise Lithiation of Gold-Coated Silicon Nanowires: A Combined In Situ Characterization and First-Principles Study. ACS Applied Materials & Eamp; Interfaces, 2015, 7, 16976-16983.   | 8.0  | 9         |
| 103 | Recent progress in first-principles simulations of anode materials and interfaces for lithium ion batteries. Current Opinion in Chemical Engineering, 2016, 13, 75-81.   | 7.8  | 9         |
| 104 | Theoretical evaluation of ethylene carbonate anion transport and its impact on solid electrolyte interphase formation. Electrochimica Acta, 2018, 266, 326-331.  | 5.2  | 9         |
| 105 | Theoretical evaluation of thermal decomposition of dichlorosilane for plasma-enhanced atomic layer deposition of silicon nitride: the important role of surface hydrogen. Physical Chemistry Chemical Physics, 2018, 20, 29152-29158.                    | 2.8  | 9         |
| 106 | Boron diffusion in strained Si:â€fA first-principles study. Journal of Applied Physics, 2004, 96, 5543-5547.   | 2.5  | 8         |
| 107 | Two-dimensional arrangement of CH3NH2 adsorption on Si(0 0 1)-2 $\tilde{A}$ — 1. Chemical Physics Letters, 2004, 385, 144-148.   | 2.6  | 8         |
| 108 | Formation and structure of vacancy defects in silicon: Combined Metropolis Monte Carlo, tight-binding molecular dynamics, and density functional theory calculations. Physical Review B, 2009, 80, .   | 3.2  | 8         |

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| 109 | Theoretical characterization of silicon self-interstitial clusters in uniform strain fields. Physical Review B, 2009, 80, .   | 3.2 | 8         |
| 110 | Prediction of the formation of stable periodic self-interstitial cluster chains [(I4)m,m=1–4] in Si under biaxial strain. Applied Physics Letters, 2009, 94, 264101.  | 3.3 | 8         |
| 111 | Revisit to the Ising model for order–disorder phase transition on Si(001). Surface Science, 2004, 554, 150-158.   | 1.9 | 7         |
| 112 | Mechanisms of monovacancy annihilation and type-A defect creation on Si(001)–2×1. Surface Science, 2004, 555, 187-192.  | 1.9 | 7         |
| 113 | Integrated atomistic modelling of interstitial defect growth in silicon. Molecular Simulation, 2009, 35, 867-879.   | 2.0 | 7         |
| 114 | First-Principles Assessment of Anomalous Thermal Degradation of Aqueous 2-Amino-2-methyl-1-propanol for CO <sub>2</sub> Capture. Energy & E | 5.1 | 7         |
| 115 | Function of subsurface boron on Si(001)-2×1: water adsorption. Surface Science, 2003, 547, L882-L886.   | 1.9 | 6         |
| 116 | Role of structural disorder in optical absorption in silicon. Physical Review B, 2010, 82, .  | 3.2 | 6         |
| 117 | On the Importance of Regulating Hydroxyl Coverage on the Basal Plane of Graphene Oxide for Supercapacitors. ChemElectroChem, 2016, 3, 741-748.  | 3.4 | 6         |
| 118 | Molecular dynamics investigation of reduced ethylene carbonate aggregation at the onset of solid electrolyte interphase formation. Physical Chemistry Chemical Physics, 2019, 21, 22449-22455.  | 2.8 | 5         |
| 119 | Strain effects on the stability and structure of vacancy clusters in Si: A first-principles study. Physical Review B, 2010, 81, .   | 3.2 | 4         |
| 120 | Role of different Pd/Pt ensembles in determining CO chemisorption on Au-based bimetallic alloys: A first-principles study. Applied Surface Science, 2015, 332, 409-418.   | 6.1 | 4         |
| 121 | Agent molecule modulated low-temperature activation of solid-state lithium-ion transport for polymer electrolytes. Journal of Power Sources, 2021, 505, 229917.   | 7.8 | 4         |
| 122 | Intriguing Thermal Degradation Behavior of Aqueous Piperazine for Carbon Dioxide Capture: A First-Principles Assessment. ACS Sustainable Chemistry and Engineering, 2022, 10, 9584-9590.  | 6.7 | 4         |
| 123 | Effects of Subsurface Boron and Phosphorus on Surface Reactivity of Si(001):Â Water and Ammonia Adsorption. Journal of Physical Chemistry B, 2004, 108, 16147-16153.  | 2.6 | 3         |
| 124 | Interstitial-based boron diffusion dynamics in amorphous silicon. Applied Physics Letters, 2008, 93, .  | 3.3 | 3         |
| 125 | Formation, nature, and stability of the arsenic-silicon-oxygen alloy for plasma doping of non-planar silicon structures. Applied Physics Letters, 2014, 105, 262102.  | 3.3 | 3         |
| 126 | First-Principles Mechanistic Study of the Initial Growth of SrO by Atomic Layer Deposition on TiO2-Terminated SrTiO3 (001). Journal of Physical Chemistry C, 2020, 124, 28116-28122.  | 3.1 | 3         |

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|-----|---|-----|-----------|
| 127 | Arsenic defect complexes atSiO2/Siinterfaces: A density functional theory study. Physical Review B, 2009, 80, .   | 3.2 | 2         |
| 128 | Defectâ€Assisted Covalent Binding of Graphene to an Amorphous Silica Surface: A Theoretical Prediction. ChemPhysChem, 2011, 12, 2155-2159.  | 2.1 | 2         |
| 129 | First-principles description of electrocatalytic characteristics of graphene-like materials. Journal of Chemical Physics, 2020, 153, 214704.  | 3.0 | 2         |
| 130 | Strong thermal conductivity dependence on arsenic-vacancy complex formation in arsenic-doped silicon. Journal of Applied Physics, 2019, 126, 195104.  | 2.5 | 1         |
| 131 | Kinetic Selectivity of Lithium Alkyl Carbonate Formation from Combination Reactions of Ethylene Carbonate Radical Anions. Journal of Physical Chemistry C, 2020, 124, 25754-25759.                | 3.1 | 1         |
| 132 | First-principles prediction on antimony-doping effects on the cyclic stability of tin anodes for lithium-ion batteries. Physical Chemistry Chemical Physics, 2022, 24, 17542-17546.               | 2.8 | 1         |
| 133 | Behavior of Si Interstitials and Boron-Interstitial Pairs at the Si/SiO2 Interface. Materials Research Society Symposia Proceedings, 2004, 810, 398.  | 0.1 | 0         |
| 134 | Diffusion of Fluorine-Silicon Interstitial Complex in Crystalline Silicon. Materials Research Society Symposia Proceedings, 2005, 864, 911.   | 0.1 | 0         |
| 135 | Role of Interstitials in As TED and Clustering in Crystalline Silicon. Materials Research Society Symposia Proceedings, 2005, 864, 851.   | 0.1 | 0         |
| 136 | Tunnel oxide thickness dependence of activation energy for SiGe quantum dot flash memory. , 2005, , .   |     | 0         |
| 137 | Understanding of the Synthesis and Structure of Si Nanocrystals in an Oxide Matrix from First Principles Based Atomistic Modeling. Materials Research Society Symposia Proceedings, 2006, 958, 1. | 0.1 | 0         |
| 138 | Ab-Initio Study of Boron Diffusion Retardation in Si1-xGex. Materials Research Society Symposia Proceedings, 2006, 912, 1.  | 0.1 | 0         |
| 139 | Multiscale Modeling of Growth and Structure of Silicon Nanoparticles in an Oxide Matrix. Materials Research Society Symposia Proceedings, 2006, 978, .  | 0.1 | 0         |
| 140 | Mechanisms for Interstitial-Mediated Transient Enhanced Diffusion of N-type Dopants. Materials Research Society Symposia Proceedings, 2006, 912, 1.   | 0.1 | 0         |
| 141 | An Experimental and Simulation Study of Arsenic Diffusion Behavior in Point Defect Engineered Silicon. Materials Research Society Symposia Proceedings, 2007, 994, 1.                             | 0.1 | 0         |
| 142 | Chemical Routes to Ultra Thin Films for Copper Barriers and Liners. Materials Research Society Symposia Proceedings, 2007, 990, 1.  | 0.1 | 0         |
| 143 | First-Principles Prediction of Optical Absorption Enhancement for Si Native Defect Clusters under Biaxial Strain. Electrochemical and Solid-State Letters, 2011, 14, P1.                          | 2.2 | 0         |
| 144 | Fundamental insight into control of thermal conductivity in silicon-germanium alloy nanowires. Materials Research Society Symposia Proceedings, 2014, 1707, 31.                                   | 0.1 | 0         |

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| 145 | Materials science of Ru and Ru alloy thin films for barrier applications. , 2016, , .  |      | O         |
| 146 | Fundamentals of Capacitive Charge Storage in Carbon-Based Supercapacitors. Springer Series in Materials Science, 2021, , 559-586.                              | 0.6  | 0         |
| 147 | Silicon-based anode materials for lithium-ion batteries. Series in Materials Science and Engineering, 2017, , 443-460.   | 0.1  | 0         |
| 148 | Plasmonic Nanostructures: Controlling Plasmonâ€Enhanced Fluorescence via Intersystem Crossing in Photoswitchable Molecules (Small 38/2017). Small, 2017, 13, . | 10.0 | O         |