

# Stefano Baroni

## List of Publications by Year in Descending Order

**Source:** <https://exaly.com/author-pdf/1287385/stefano-baroni-publications-by-year.pdf>

**Version:** 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

216  
papers

30,898  
citations

50  
h-index

175  
g-index

220  
ext. papers

35,270  
ext. citations

4.5  
avg. IF

6.58  
L-index

| #   | Paper  | IF   | Citations |
|-----|--|------|-----------|
| 216 | Inflammatory and metabolic markers in patients with mood disorders. <i>World Journal of Biological Psychiatry</i> , <b>2021</b> , 22, 228-235  | 3.8  | 2         |
| 215 | Heat transport in liquid water from first-principles and deep neural network simulations. <i>Physical Review B</i> , <b>2021</b> , 104,  | 3.3  | 4         |
| 214 | Thermal and Tidal Evolution of Uranus with a Growing Frozen Core. <i>Planetary Science Journal</i> , <b>2021</b> , 2, 222  | 2.9  | 5         |
| 213 | Discovery of a natural cyan blue: A unique food-sourced anthocyanin could replace synthetic brilliant blue. <i>Science Advances</i> , <b>2021</b> , 7,   | 14.3 | 8         |
| 212 | Decreased Plasma Oxytocin Levels in Patients With PTSD. <i>Frontiers in Psychology</i> , <b>2021</b> , 12, 612338  | 3.4  | 2         |
| 211 | Cariprazine as a therapeutic option for schizophrenia: a drug evaluation. <i>Expert Opinion on Pharmacotherapy</i> , <b>2021</b> , 22, 415-426   | 4    | 2         |
| 210 | Invariance principles in the theory and computation of transport coefficients. <i>European Physical Journal B</i> , <b>2021</b> , 94, 160  | 1.2  | 3         |
| 209 | QEHeat: An open-source energy flux calculator for the computation of heat-transport coefficients from first principles. <i>Computer Physics Communications</i> , <b>2021</b> , 269, 108090                 | 4.2  | 3         |
| 208 | State-of-the-Art: Inflammatory and Metabolic Markers in Mood Disorders. <i>Life</i> , <b>2020</b> , 10,  | 3    | 6         |
| 207 | Effectiveness of clozapine, oxcarbazepine and rivastigmine combination in a bipolar disorder patient with initial cerebral atrophy. <i>Clinical Case Reports (discontinued)</i> , <b>2020</b> , 8, 254-257 | 0.7  | 1         |
| 206 | Heat and charge transport in HO at ice-giant conditions from ab initio molecular dynamics simulations. <i>Nature Communications</i> , <b>2020</b> , 11, 3605   | 17.4 | 8         |
| 205 | Oxidation States, ThoulessPumps, and Nontrivial Ionic Transport in Nonstoichiometric Electrolytes. <i>Physical Review X</i> , <b>2020</b> , 10,  | 9.1  | 3         |
| 204 | Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. <i>Physical Review B</i> , <b>2020</b> , 102,   | 3.3  | 1         |
| 203 | The complex interactions among serotonin, insulin, leptin, and glycolipid metabolic parameters in human obesity. <i>CNS Spectrums</i> , <b>2020</b> , 1-10   | 1.8  | 3         |
| 202 | Psychopharmacology and ethnicity: A comparative study on Senegalese and Italian men. <i>World Journal of Biological Psychiatry</i> , <b>2020</b> , 21, 300-307   | 3.8  | 1         |
| 201 | The Relationships Between Obsessive-Compulsive Disorder and Psychosis: An Unresolved Issue. <b>2020</b> , 17, 149-157  |      | 0         |
| 200 | Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach. <i>Nature Communications</i> , <b>2019</b> , 10, 3853   | 17.4 | 39        |

|     |  |      |    |
|-----|--|------|----|
| 199 | Fast hybrid density-functional computations using plane-wave basis sets. <i>Electronic Structure</i> , <b>2019</b> , 1, 015009   | 2.6  | 16 |
| 198 | Unraveling the molecular mechanisms of color expression in anthocyanins. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 8757-8766  | 3.6  | 10 |
| 197 | Treatment of the obsessive-compulsive and bipolar disorders comorbidity: pharmacodynamic and pharmacokinetic evaluation. <i>Expert Opinion on Drug Metabolism and Toxicology</i> , <b>2019</b> , 15, 619-631 | 5.5  | 3  |
| 196 | Topological quantization and gauge invariance of charge transport in liquid insulators. <i>Nature Physics</i> , <b>2019</b> , 15, 967-972  | 16.2 | 14 |
| 195 | Sex-Related Differences in Plasma Oxytocin Levels in Humans. <i>Clinical Practice and Epidemiology in Mental Health</i> , <b>2019</b> , 15, 58-63  | 3.2  | 24 |
| 194 | Problematic Internet use in drug addicts under treatment in public rehab centers. <i>World Journal of Psychiatry</i> , <b>2019</b> , 9, 55-64  | 3    | 7  |
| 193 | Emotional Blunting, Cognitive Impairment, Bone Fractures, and Bleeding as Possible Side Effects of Long-Term Use of SSRIs. <b>2019</b> , 16, 75-85   |      |    |
| 192 | Effect of Valproate and Antidepressant Drugs on Clozapine Metabolism in Patients With Psychotic Mood Disorders. <i>Therapeutic Drug Monitoring</i> , <b>2018</b> , 40, 443-451                               | 3.2  | 7  |
| 191 | Spin dynamics from time-dependent density functional perturbation theory. <i>European Physical Journal B</i> , <b>2018</b> , 91, 1   | 1.2  | 7  |
| 190 | Ab initio study of electron energy loss spectra of bulk bismuth up to 100 eV. <i>Physical Review B</i> , <b>2017</b> , 95,   | 3.3  | 4  |
| 189 | Decreased lymphocyte dopamine transporter in romantic lovers. <i>CNS Spectrums</i> , <b>2017</b> , 22, 290-294   | 1.8  | 8  |
| 188 | Accurate thermal conductivities from optimally short molecular dynamics simulations. <i>Scientific Reports</i> , <b>2017</b> , 7, 15835  | 4.9  | 28 |
| 187 | Microscopic theory and quantum simulation of atomic heat transport. <i>Nature Physics</i> , <b>2016</b> , 12, 80-84  | 16.2 | 63 |
| 186 | Sampling Molecular Conformers in Solution with Quantum Mechanical Accuracy at a Nearly Molecular-Mechanics Cost. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 4385-9                | 6.4  | 14 |
| 185 | Multimodel Approach to the Optical Properties of Molecular Dyes in Solution. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 4423-9  | 6.4  | 10 |
| 184 | Gauge Invariance of Thermal Transport Coefficients. <i>Journal of Low Temperature Physics</i> , <b>2016</b> , 185, 79-863  |      | 19 |
| 183 | Current Trends on Antipsychotics: Focus on Asenapine. <i>Current Medicinal Chemistry</i> , <b>2016</b> , 23, 2204-16   | 4.3  | 12 |
| 182 | Effectiveness of Nalmefene in Binge Eating Disorder: A Case Report. <i>Journal of Clinical Psychopharmacology</i> , <b>2016</b> , 36, 103-4  | 1.7  | 4  |

|     |   |     |    |
|-----|---|-----|----|
| 181 | Asenapine augmentation in bipolar disorders: a case series. <i>Clinical Case Reports (discontinued)</i> , <b>2016</b> , 4, 499-504  | 0.7 | 4  |
| 180 | Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 034111   | 3.9 | 14 |
| 179 | Accurate and inexpensive prediction of the color optical properties of anthocyanins in solution. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 3816-22  | 2.8 | 28 |
| 178 | Neurobiological correlates of social anxiety disorder: an update. <i>CNS Spectrums</i> , <b>2015</b> , 20, 100-11   | 1.8 | 29 |
| 177 | Optical properties of anthocyanins in the gas phase. <i>Chemical Physics Letters</i> , <b>2015</b> , 618, 24-29   | 2.5 | 3  |
| 176 | Plasma Oxytocin Levels in Untreated Adult Obsessive-Compulsive Disorder Patients. <i>Neuropsychobiology</i> , <b>2015</b> , 72, 74-80   | 4   | 23 |
| 175 | Neuropsychological Testing in Interventional Cardiology Staff after Long-Term Exposure to Ionizing Radiation. <i>Journal of the International Neuropsychological Society</i> , <b>2015</b> , 21, 670-6  | 3.1 | 31 |
| 174 | turboEELS code for the simulation of the electron energy loss and inelastic X-ray scattering spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , <b>2015</b> , 196, 460-469 | 4.2 | 23 |
| 173 | Food addiction spectrum: a theoretical model from normality to eating and overeating disorders. <i>Current Medicinal Chemistry</i> , <b>2015</b> , 22, 1631-8   | 4.3 | 15 |
| 172 | Nalmefene: A Novel Drug for an Old Disorder. <i>Current Medicinal Chemistry</i> , <b>2015</b> , 22, 3162-8  | 4.3 | 2  |
| 171 | The inflammatory hypothesis of mood spectrum broadened to fibromyalgia and chronic fatigue syndrome. <i>Clinical and Experimental Rheumatology</i> , <b>2015</b> , 33, S109-16  | 2.2 | 11 |
| 170 | Dimorphic changes of some features of loving relationships during long-term use of antidepressants in depressed outpatients. <i>Journal of Affective Disorders</i> , <b>2014</b> , 166, 151-5   | 6.6 | 7  |
| 169 | Behavioral addictions: a novel challenge for psychopharmacology. <i>CNS Spectrums</i> , <b>2014</b> , 19, 486-95  | 1.8 | 24 |
| 168 | Approximate treatment of semicore states in GW calculations with application to Au clusters. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 124101   | 3.9 | 5  |
| 167 | Clozapine effects on adenylyl cyclase activity and serotonin type 1A receptors in human brain post-mortem. <i>Journal of Psychopharmacology</i> , <b>2014</b> , 28, 320-8   | 4.6 | 5  |
| 166 | Metabolic syndrome and major depression. <i>CNS Spectrums</i> , <b>2014</b> , 19, 293-304   | 1.8 | 98 |
| 165 | turboTDDFT 2.0: hybrid functionals and new algorithms within time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , <b>2014</b> , 185, 2080-2089   | 4.2 | 43 |
| 164 | Pathological gambling and impulsivity: an Italian study. <i>Rivista Di Psichiatria</i> , <b>2014</b> , 49, 95-9   | 3.1 | 13 |

|     |  |     |    |
|-----|--|-----|----|
| 163 | Energy-level alignment in organic dye-sensitized TiO <sub>2</sub> from GW calculations. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 014709   | 3.9 | 43 |
| 162 | Electron energy loss and inelastic x-ray scattering cross sections from time-dependent density-functional perturbation theory. <i>Physical Review B</i> , <b>2013</b> , 88,  | 3.3 | 19 |
| 161 | Serotonin receptor of type 6 (5-HT <sub>6</sub> ) in human prefrontal cortex and hippocampus post-mortem: an immunohistochemical and immunofluorescence study. <i>Neurochemistry International</i> , <b>2013</b> , 62, 182-8 | 4.4 | 27 |
| 160 | The neurobiology of moral sense: facts or hypotheses?. <i>Annals of General Psychiatry</i> , <b>2013</b> , 12, 6   | 3.4 | 21 |
| 159 | Glutamate system as target for development of novel antidepressants. <i>CNS Spectrums</i> , <b>2013</b> , 18, 188-98   | 1.8 | 21 |
| 158 | The expression of platelet serotonin transporter (SERT) in human obesity. <i>BMC Neuroscience</i> , <b>2013</b> , 14, 128  | 3.2 | 12 |
| 157 | Pharmacokinetics and pharmacodynamics of psychotropic drugs: effect of sex. <i>CNS Spectrums</i> , <b>2013</b> , 18, 118-27  | 1.8 | 48 |
| 156 | Non-Monoaminergic Targets for the Development of Antidepressants: Focus on Neuropeptides. <i>Mini-Reviews in Medicinal Chemistry</i> , <b>2013</b> , 13, 2-10  | 3.2 | 24 |
| 155 | Serotonin Receptors of Type 6 (5-HT <sub>6</sub> ): From Neuroscience to Clinical Pharmacology. <i>Current Medicinal Chemistry</i> , <b>2013</b> , 20, 371-377   | 4.3 | 16 |
| 154 | Prefrontal cortex, dopamine, and jealousy endophenotype. <i>CNS Spectrums</i> , <b>2013</b> , 18, 6-14   | 1.8 | 16 |
| 153 | The relationship between epilepsy and depression: an update. <i>Current Medicinal Chemistry</i> , <b>2013</b> , 20, 2861-7   | 4.3 | 10 |
| 152 | The role of platelet/lymphocyte serotonin transporter in depression and beyond. <i>Current Drug Targets</i> , <b>2013</b> , 14, 522-30   | 3   | 12 |
| 151 | A link between oxytocin and serotonin in humans: supporting evidence from peripheral markers. <i>European Neuropsychopharmacology</i> , <b>2012</b> , 22, 578-83   | 1.2 | 23 |
| 150 | Plasma fluvoxamine levels and OCD symptoms/response in adult patients. <i>Human Psychopharmacology</i> , <b>2012</b> , 27, 397-402   | 2.3 | 5  |
| 149 | Distribution of serotonin receptor of type 6 (5-HT <sub>6</sub> ) in human brain post-mortem. A pharmacology, autoradiography and immunohistochemistry study. <i>Neurochemical Research</i> , <b>2012</b> , 37, 920-7        | 4.6 | 22 |
| 148 | Cognitive, psychological and psychiatric effects of ionizing radiation exposure. <i>Current Medicinal Chemistry</i> , <b>2012</b> , 19, 1864-9   | 4.3 | 41 |
| 147 | Absolute transition rates for rare events from dynamical decoupling of reaction variables. <i>Physical Review Letters</i> , <b>2012</b> , 109, 150601  | 7.4 | 8  |
| 146 | Plasma clomipramine levels in adult patients with obsessive-compulsive disorder. <i>International Clinical Psychopharmacology</i> , <b>2012</b> , 27, 55-60  | 2.2 | 6  |

|     |  |      |     |
|-----|--|------|-----|
| 145 | Gender effect on the relationship between stress hormones and panic-agoraphobic spectrum dimensions in healthy subjects. <i>CNS Spectrums</i> , <b>2012</b> , 17, 214-20   | 1.8  | 5   |
| 144 | Serotonin receptors of type 6 (5-HT <sub>6</sub> ): what can we expect from them?. <i>Current Medicinal Chemistry</i> , <b>2011</b> , 18, 2783-90  | 4.3  | 20  |
| 143 | Itinerant ferromagnetic phase of the Hubbard model. <i>Physical Review B</i> , <b>2011</b> , 83,   | 3.3  | 21  |
| 142 | Surface Precursors and Reaction Mechanisms for the Thermal Reduction of Graphene Basal Surfaces Oxidized by Atomic Oxygen. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 4730-4737                               | 3.8  | 82  |
| 141 | Oxygen dissociation by concerted action of di-iron centers in metal-organic coordination networks at surfaces: modeling non-heme iron enzymes. <i>Nano Letters</i> , <b>2011</b> , 11, 5414-20                                 | 11.5 | 60  |
| 140 | Is androstadienone a putative human pheromone?. <i>Current Medicinal Chemistry</i> , <b>2011</b> , 18, 1213-9  | 4.3  | 3   |
| 139 | turboTDDFT Å code for the simulation of molecular spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , <b>2011</b> , 182, 1744-1754 | 4.2  | 133 |
| 138 | Novel treatment options of binge eating disorder. <i>Current Medicinal Chemistry</i> , <b>2011</b> , 18, 5159-64   | 4.3  | 9   |
| 137 | Latest advancements on serotonin and dopamine transporters in lymphocytes. <i>Mini-Reviews in Medicinal Chemistry</i> , <b>2010</b> , 10, 32-40  | 3.2  | 24  |
| 136 | Romantic attachment and subtypes/dimensions of jealousy. <i>Clinical Practice and Epidemiology in Mental Health</i> , <b>2010</b> , 6, 53-8  | 3.2  | 17  |
| 135 | Harnessing molecular excited states with Lanczos chains. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 074204   | 1.8  | 14  |
| 134 | Reptation quantum Monte Carlo algorithm for lattice Hamiltonians with a directed-update scheme. <i>Physical Review E</i> , <b>2010</b> , 82, 046710  | 2.4  | 11  |
| 133 | Metallization of the C <sub>60</sub> /Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations. <i>Journal of Chemical Physics</i> , <b>2010</b> , 132, 234710              | 3.9  | 4   |
| 132 | Male axillary extracts modify the affinity of the platelet serotonin transporter and impulsiveness in women. <i>Physiology and Behavior</i> , <b>2010</b> , 100, 364-8   | 3.5  | 8   |
| 131 | Alterations of the dopamine transporter in resting lymphocytes of patients with different psychotic disorders. <i>Psychiatry Research</i> , <b>2010</b> , 175, 54-7  | 9.9  | 15  |
| 130 | GW quasiparticle spectra from occupied states only. <i>Physical Review B</i> , <b>2010</b> , 81,   | 3.3  | 155 |
| 129 | Order-disorder phase boundary between ice VII and VIII obtained by first principles. <i>Chemical Physics Letters</i> , <b>2010</b> , 499, 236-240  | 2.5  | 30  |
| 128 | Impulsivity, gender, and the platelet serotonin transporter in healthy subjects. <i>Neuropsychiatric Disease and Treatment</i> , <b>2010</b> , 6, 9-15   | 3.1  | 20  |

|     |   |      |       |
|-----|---|------|-------|
| 127 | Zero-temperature dynamics of solid H4e from quantum Monte Carlo simulations. <i>Physical Review B</i> , <b>2009</b> , 80,   | 3.3  | 8     |
| 126 | Second messenger modulation: a novel target of future antidepressants?. <i>Current Medicinal Chemistry</i> , <b>2009</b> , 16, 4679-90  | 4.3  | 5     |
| 125 | Time-dependent density functional theory study of squaraine dye-sensitized solar cells. <i>Chemical Physics Letters</i> , <b>2009</b> , 475, 49-53  | 2.5  | 79    |
| 124 | QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 395502  | 1.8  | 13251 |
| 123 | [(3)H]-YM-09151-2 binding sites in human brain postmortem. <i>Neurochemistry International</i> , <b>2009</b> , 55, 643-7  | 4.4  | 10    |
| 122 | Normalisation of immune cell imbalance after pharmacological treatments of patients suffering from obsessive-compulsive disorder. <i>Journal of Psychopharmacology</i> , <b>2009</b> , 23, 567-73                   | 4.6  | 16    |
| 121 | Optimal representation of the polarization propagator for large-scale GW calculations. <i>Physical Review B</i> , <b>2009</b> , 79,   | 3.3  | 95    |
| 120 | Molecular design of photoactive acenes for organic photovoltaics. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 194701  | 3.9  | 18    |
| 119 | Adsorption of chlorine on Ag(111): No subsurface Cl at low coverage. <i>Physical Review B</i> , <b>2008</b> , 78,   | 3.3  | 33    |
| 118 | Electronic structure of surface-supported bis(phthalocyaninato) terbium(III) single molecular magnets. <i>Nano Letters</i> , <b>2008</b> , 8, 3364-8  | 11.5 | 165   |
| 117 | Ab initio simulation of photoemission spectroscopy in solids: Plane-wave pseudopotential approach with applications to normal-emission spectra of Cu(001) and Cu(111). <i>Physical Review B</i> , <b>2008</b> , 77, | 3.3  | 9     |
| 116 | Activated Adsorption of Ethylene on Atomic-Oxygen-Covered Ag(100) and Ag(210): Formation of an Oxametallacycle. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 1019-1027                               | 3.8  | 17    |
| 115 | Decreased density of the platelet serotonin transporter in pathological gamblers. <i>Neuropsychobiology</i> , <b>2008</b> , 57, 38-43   | 4    | 24    |
| 114 | Turbo charging time-dependent density-functional theory with Lanczos chains. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 154105   | 3.9  | 207   |
| 113 | Properties of Pt-supported Co nanomagnets from relativistic density functional theory calculations. <i>Physical Review B</i> , <b>2008</b> , 78,  | 3.3  | 25    |
| 112 | Presence and characterization of the dopamine transporter in human resting lymphocytes. <i>Neurochemical Research</i> , <b>2008</b> , 33, 1011-6  | 4.6  | 12    |
| 111 | Hydrogen and coordination bonding supramolecular structures of trimesic acid on Cu(110). <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 12589-603  | 2.8  | 107   |
| 110 | Computational spectroscopy of carbon monoxide isotopomers in helium clusters. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 7640-5  | 2.8  | 26    |



|     |   |      |     |
|-----|---|------|-----|
| 109 | Unraveling excited states of doped helium clusters. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 12749-53  | 2.8  | 4   |
| 108 | Presence of D4 dopamine receptors in human prefrontal cortex: a postmortem study. <i>Revista Brasileira De Psiquiatria</i> , <b>2007</b> , 29, 148-52   | 2.6  | 4   |
| 107 | SixC1 $\alpha$ O2 alloys: A possible route to stabilize carbon-based silica-like solids?. <i>Solid State Communications</i> , <b>2007</b> , 144, 273-276  | 1.6  | 14  |
| 106 | Tubby protein in human lymphocytes from normal weight and obese subjects. <i>Clinical Biochemistry</i> , <b>2007</b> , 40, 806-9  | 3.5  | 4   |
| 105 | Characterizing In and N impurities in GaAs from ab initio computer simulation of (110) cross-sectional STM images. <i>Physical Review B</i> , <b>2007</b> , 75,                                   | 3.3  | 5   |
| 104 | Thermal balneotherapy induces changes of the platelet serotonin transporter in healthy subjects. <i>Progress in Neuro-Psychopharmacology and Biological Psychiatry</i> , <b>2007</b> , 31, 1436-9 | 5.5  | 10  |
| 103 | Defect-controlled transport properties of metallic atoms along carbon nanotube surfaces. <i>Physical Review Letters</i> , <b>2007</b> , 99, 046803  | 7.4  | 26  |
| 102 | Common alterations in the serotonin transporter in platelets and lymphocytes of psychotic patients. <i>Pharmacopsychiatry</i> , <b>2006</b> , 39, 35-8  | 2    | 15  |
| 101 | A relationship between oxytocin and anxiety of romantic attachment. <i>Clinical Practice and Epidemiology in Mental Health</i> , <b>2006</b> , 2, 28  | 3.2  | 79  |
| 100 | Methane dehydrogenation on Rh@Cu(111): a first-principles study of a model catalyst. <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 12448-54                                | 16.4 | 48  |
| 99  | Cross-sectional imaging of sharp Si interlayers embedded in gallium arsenide. <i>Applied Physics Letters</i> , <b>2006</b> , 88, 022115   | 3.4  | 3   |
| 98  | Efficient approach to time-dependent density-functional perturbation theory for optical spectroscopy. <i>Physical Review Letters</i> , <b>2006</b> , 96, 113001                                   | 7.4  | 166 |
| 97  | Interaction of hydrogen with cerium oxide surfaces: a quantum mechanical computational study. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 19380-5                                 | 3.4  | 77  |
| 96  | DFT study of a weakly pi-bonded C2H4 on oxygen-covered Ag(100). <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 367-76  | 3.4  | 18  |
| 95  | Monitoring two-dimensional coordination reactions: directed assembly of co-terephthalate nanosystems on Au(111). <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 5627-32              | 3.4  | 72  |
| 94  | Binding of 3H-WIN-35,428 and 125I-RTI-121 to human platelet membranes. <i>Neurochemical Research</i> , <b>2006</b> , 31, 361-5  | 4.6  | 13  |
| 93  | Taming multiple valency with density functionals: A case study of defective ceria. <i>Physical Review B</i> , <b>2005</b> , 71,   | 3.3  | 347 |
| 92  | First-principles codes for computational crystallography in the Quantum-ESPRESSO package. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , <b>2005</b> , 220,                    | 1    | 122 |



|    |   |      |     |
|----|---|------|-----|
| 91 | Decreased density of peripheral benzodiazepine receptors in psychiatric patients after a suicide attempt. <i>Life Sciences</i> , <b>2005</b> , 77, 3268-75  | 6.8  | 7   |
| 90 | Electronic and atomistic structures of clean and reduced ceria surfaces. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 22860-7  | 3.4  | 314 |
| 89 | Reply to 'Comment on "Naming multiple valency with density functionals: A case study of defective ceria"' <i>Physical Review B</i> , <b>2005</b> , 72,  | 3.3  | 161 |
| 88 | On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. <i>Surface Science</i> , <b>2005</b> , 587, 50-54  | 1.8  | 10  |
| 87 | Computational spectroscopy of doped He clusters. <i>Computer Physics Communications</i> , <b>2005</b> , 169, 404-407.   | 4.2  | 18  |
| 86 | Characterization of Si-doped GaAs cross-sectional surfaces via ab initio simulations. <i>Physical Review B</i> , <b>2005</b> , 72,  | 3.3  | 13  |
| 85 | Computer simulation of quantum melting in hydrogen clusters. <i>ChemPhysChem</i> , <b>2005</b> , 6, 1884-8  | 3.2  | 30  |
| 84 | Templated growth of metal-organic coordination chains at surfaces. <i>Angewandte Chemie - International Edition</i> , <b>2005</b> , 44, 6142-5  | 16.4 | 118 |
| 83 | Energetically driven reorganization of a modified catalytic surface under reaction conditions. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 2351-7  | 16.4 | 27  |
| 82 | Computational spectroscopy of helium-solvated molecules: effective inertia, from small He clusters toward the nanodroplet regime. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 114306                  | 3.9  | 57  |
| 81 | Spin-flop ordering from frustrated ferro- and antiferromagnetic interactions: a combined theoretical and experimental study of a Mn/Fe(100) monolayer. <i>Physical Review Letters</i> , <b>2005</b> , 95, 117207. | 7.4  | 26  |
| 80 | Changes in peripheral benzodiazepine receptors in patients with bipolar disorder. <i>Neuropsychiatric Disease and Treatment</i> , <b>2005</b> , 1, 151-4  | 3.1  | 3   |
| 79 | Anomalous pressure-induced transition(s) in ice XI. <i>Physical Review Letters</i> , <b>2004</b> , 92, 105502   | 7.4  | 35  |
| 78 | Absence of NK1 receptors in human blood lymphocytes and granulocytes. <i>Neuropsychobiology</i> , <b>2004</b> , 50, 221-5   | 4    | 2   |
| 77 | Platelet alpha2-adrenoreceptors in obsessive-compulsive disorder. <i>Neuropsychobiology</i> , <b>2004</b> , 49, 81-3  | 4    | 3   |
| 76 | Adsorption of ethylene on stepped Ag() surfaces. <i>Surface Science</i> , <b>2004</b> , 566-568, 1018-1023  | 1.8  | 15  |
| 75 | Engineering the reactivity of metal catalysts: a model study of methane dehydrogenation on Rh(111). <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 16732-3                                  | 16.4 | 63  |
| 74 | Rotational dynamics of CO solvated in small He clusters: a quantum Monte Carlo study. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 9071-6  | 3.9  | 45  |

|    |   |      |      |
|----|---|------|------|
| 73 | Platelet serotonin transporter in patients with diarrhea-predominant irritable bowel syndrome both before and after treatment with alosetron. <i>American Journal of Gastroenterology</i> , <b>2003</b> , 98, 2705-11 | 0.7  | 49   |
| 72 | Oxygen vibrations in O <sub>2</sub> /Ag(0 0 1). <i>Surface Science</i> , <b>2003</b> , 530, 26-36   | 1.8  | 13   |
| 71 | Co-adsorption of ethylene and oxygen on the Ag(001) surface. <i>Surface Science</i> , <b>2003</b> , 532-535, 191-197  | 1.8  | 14   |
| 70 | Normal and obsessional jealousy: a study of a population of young adults. <i>European Psychiatry</i> , <b>2003</b> , 18, 106-11   | 6    | 32   |
| 69 | Jealousy and subthreshold psychopathology: a serotonergic link. <i>Neuropsychobiology</i> , <b>2003</b> , 47, 12-6  | 4    | 14   |
| 68 | Decreased lymphocyte 3H-paroxetine binding in obsessive-compulsive disorder. <i>Neuropsychobiology</i> , <b>2003</b> , 47, 128-30   | 4    | 4    |
| 67 | Structure, rotational dynamics, and superfluidity of small OCS-doped He clusters. <i>Physical Review Letters</i> , <b>2003</b> , 90, 143401   | 7.4  | 104  |
| 66 | Decreased inhibitory activity of PKC in OCD patients after six months of treatment. <i>Psychoneuroendocrinology</i> , <b>2002</b> , 27, 769-76  | 5    | 10   |
| 65 | The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 9839-9846  | 3.4  | 43   |
| 64 | Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. <i>Surface Science</i> , <b>2002</b> , 501, 182-190  | 1.8  | 42   |
| 63 | Distribution of [3H]GR65630 binding in human brain postmortem. <i>Neurochemical Research</i> , <b>2001</b> , 26, 187-90   | 4.6  | 18   |
| 62 | Correlation between platelet alpha(2)-adrenoreceptors and symptom severity in major depression. <i>Neuropsychobiology</i> , <b>2001</b> , 44, 122-5   | 4    | 7    |
| 61 | Pharmacological characterization of the serotonin transporter in young and elderly subjects. <i>Neuropsychobiology</i> , <b>2001</b> , 44, 78-83  | 4    | 5    |
| 60 | Phonons and related crystal properties from density-functional perturbation theory. <i>Reviews of Modern Physics</i> , <b>2001</b> , 73, 515-562  | 40.5 | 5812 |
| 59 | First principles thermoelasticity of MgSiO <sub>3</sub> -perovskite: Consequences for the inferred properties of the lower mantle. <i>Geophysical Research Letters</i> , <b>2001</b> , 28, 2699-2702                  | 4.9  | 49   |
| 58 | Decreased platelet [3H]paroxetine binding sites in suicide attempters. <i>Psychiatry Research</i> , <b>2001</b> , 103, 125-31   | 9.9  | 13   |
| 57 | Oxygen self-diffusion in alpha-quartz. <i>Physical Review Letters</i> , <b>2001</b> , 86, 4564-7  | 7.4  | 56   |
| 56 | Increased density of the platelet serotonin transporter in autism. <i>Pharmacopsychiatry</i> , <b>2000</b> , 33, 165-8  | 2    | 38   |

|    |  |     |     |
|----|--|-----|-----|
| 55 | Effects of isotopic disorder on the Raman spectra of crystals: Theory and ab initio calculations for diamond and germanium. <i>Physical Review B</i> , <b>2000</b> , 61, 9387-9392   | 3.3 | 18  |
| 54 | Magnons in real materials from density-functional theory. <i>Physical Review B</i> , <b>2000</b> , 61, R6459-R6462   | 3.3 | 85  |
| 53 | Effects of isotopic disorder on the Raman spectra of crystals: theory and ab initio calculations for diamond and germanium. <i>Computational Materials Science</i> , <b>2000</b> , 17, 395-399   | 3.2 | 7   |
| 52 | Thermodynamic properties and lattice dynamics of silver at high pressure: A first-principles study. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , <b>1999</b> , 79, 911-919 |     | 15  |
| 51 | Reptation Quantum Monte Carlo: A Method for Unbiased Ground-State Averages and Imaginary-Time Correlations. <i>Physical Review Letters</i> , <b>1999</b> , 82, 4745-4748   | 7.4 | 184 |
| 50 | Effects of disorder on the optical gap of (Zn,Mg)(S,Se). <i>Applied Physics Letters</i> , <b>1999</b> , 75, 2746-2748  | 3.4 | 13  |
| 49 | High-pressure thermal expansion, bulk modulus, and phonon structure of diamond. <i>Physical Review B</i> , <b>1999</b> , 60, 9444-9449   | 3.3 | 70  |
| 48 | Temperature-dependent surface relaxations of Ag(111). <i>Physical Review B</i> , <b>1999</b> , 59, 970-974   | 3.3 | 53  |
| 47 | Platelet [3H]paroxetine binding in patients with OCD-related disorders. <i>Psychiatry Research</i> , <b>1999</b> , 89, 223-8   | 9.9 | 31  |
| 46 | The reconstruction of nickel and rhodium (001) surfaces upon carbon, nitrogen or oxygen adsorptions. <i>Surface Science</i> , <b>1999</b> , 437, 18-28   | 1.8 | 36  |
| 45 | First-principles calculation of the thermal properties of silver. <i>Physical Review B</i> , <b>1999</b> , 59, 965-969   | 3.3 | 109 |
| 44 | Presence and characterization of the serotonin transporter in human resting lymphocytes. <i>Neuropsychopharmacology</i> , <b>1998</b> , 19, 154-9  | 8.7 | 23  |
| 43 | <del>B</del> - $\beta$ phase transition in tin: A theoretical study based on density-functional perturbation theory. <i>Physical Review B</i> , <b>1998</b> , 57, 10421-10423  | 3.3 | 86  |
| 42 | Dynamical-charge neutrality at a crystal surface. <i>Physical Review B</i> , <b>1998</b> , 57, 5742-5745   | 3.3 | 16  |
| 41 | Vibrational broadening of x-ray emission spectra: A first-principles study on diamond. <i>Physical Review B</i> , <b>1997</b> , 55, 9649-9658  | 3.3 | 19  |
| 40 | The surface chemistry of metal-oxygen interactions: a first-principles study of O:Rh(110). <i>Surface Science</i> , <b>1997</b> , 370, 166-178   | 1.8 | 33  |
| 39 | The structure and phase stability of CO adsorbates on Rh(110). <i>Surface Science</i> , <b>1997</b> , 382, L666-L671   | 1.8 | 8   |
| 38 | Theory of the Anomalous Rayleigh Dispersion at H/W(110) Surfaces. <i>Physical Review Letters</i> , <b>1996</b> , 77, 2491-2494   | 7.4 | 50  |

|    |   |     |     |
|----|---|-----|-----|
| 37 | The phonon spectra of LiH and LiD from density-functional perturbation theory. <i>Solid State Communications</i> , <b>1996</b> , 98, 203-207  | 1.6 | 30  |
| 36 | InAs/GaSb(001) valence-band offset: Independence of interface composition and strain. <i>Applied Physics Letters</i> , <b>1996</b> , 69, 3218-3220  | 3.4 | 12  |
| 35 | High-pressure low-symmetry phases of cesium halides. <i>Physical Review B</i> , <b>1995</b> , 51, 8060-8068   | 3.3 | 22  |
| 34 | Anharmonic Phonon Lifetimes in Semiconductors from Density-Functional Perturbation Theory. <i>Physical Review Letters</i> , <b>1995</b> , 75, 1819-1822                                       | 7.4 | 270 |
| 33 | Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. <i>Physical Review B</i> , <b>1994</b> , 49, 5323-5328                                      | 3.3 | 81  |
| 32 | Bulk and interfacial strain in Si/Ge heterostructures. <i>Physical Review B</i> , <b>1994</b> , 49, 7490-7498   | 3.3 | 22  |
| 31 | Structure and phase stability of $GaxIn_{1-x}P$ solid solutions from computational alchemy. <i>Physical Review Letters</i> , <b>1994</b> , 72, 4001-4004                                      | 7.4 | 56  |
| 30 | Vibrational and dielectric properties of C60 from density-functional perturbation theory. <i>Journal of Chemical Physics</i> , <b>1994</b> , 100, 8537-8539                                   | 3.9 | 150 |
| 29 | Dependence of the crystal lattice constant on isotopic composition: Theory and ab initio calculations for C, Si, and Ge. <i>Solid State Communications</i> , <b>1994</b> , 90, 295-297        | 1.6 | 81  |
| 28 | Third-order density-functional perturbation theory: A practical implementation with applications to anharmonic couplings in Si. <i>Solid State Communications</i> , <b>1994</b> , 91, 813-816 | 1.6 | 41  |
| 27 | Nonlinear piezoelectricity in CdTe. <i>Physical Review B</i> , <b>1993</b> , 47, 16252-16256  | 3.3 | 41  |
| 26 | Ab initio calculation of the band offset at strained GaAs/InAs (001) heterojunctions. <i>Physical Review B</i> , <b>1993</b> , 48, 17607-17610  | 3.3 | 35  |
| 25 | Auxiliary-field quantum Monte Carlo calculations for systems with long-range repulsive interactions. <i>Physical Review Letters</i> , <b>1993</b> , 71, 1148-1151                             | 7.4 | 28  |
| 24 | Ab initio calculation of phonon dispersions in II-VI semiconductors. <i>Physical Review B</i> , <b>1993</b> , 47, 3588-3592   | 3.3 | 196 |
| 23 | Phonon softening and high-pressure low-symmetry phases of cesium iodide. <i>Physical Review Letters</i> , <b>1992</b> , 69, 1069-1072   | 7.4 | 27  |
| 22 | Effects of disorder on the Raman spectra of GaAs/AlAs superlattices. <i>Physical Review B</i> , <b>1992</b> , 45, 4280-4288   | 3.3 | 87  |
| 21 | Effects of disorder on the vibrational properties of SiGe alloys: Failure of mean-field approximations. <i>Physical Review Letters</i> , <b>1992</b> , 69, 1959-1962                          | 7.4 | 38  |
| 20 | Atomic intermixing in short period GaAs/AlAs superlattices. <i>Surface Science</i> , <b>1992</b> , 267, 171-175   | 1.8 | 24  |

|    |  |     |      |
|----|--|-----|------|
| 19 | Vibrational properties of isolated AlAs monolayers embedded in GaAs: a theoretical study of the effects of disorder. <i>Applied Surface Science</i> , <b>1992</b> , 56-58, 617-621 | 6.7 |      |
| 18 | Tuning band offsets at semiconductor interfaces by intralayer deposition. <i>Physical Review B</i> , <b>1991</b> , 43, 7347-7350   | 3.3 | 98   |
| 17 | Structure and thermodynamics of SixGe1-x alloys from ab initio Monte Carlo simulations. <i>Physical Review Letters</i> , <b>1991</b> , 66, 2116-2119                               | 7.4 | 144  |
| 16 | Ab initio calculation of phonon dispersions in semiconductors. <i>Physical Review B</i> , <b>1991</b> , 43, 7231-7242  | 3.3 | 1348 |
| 15 | Phonon spectra of ultrathin GaAs/AlAs superlattices: An ab initio calculation. <i>Physical Review B</i> , <b>1990</b> , 41, 3870-3873  | 3.3 | 110  |
| 14 | Phonon dispersions in GaxAl1-xAs alloys. <i>Physical Review Letters</i> , <b>1990</b> , 65, 84-87  | 7.4 | 104  |
| 13 | Electronic structure of InP/Ga0.47In0.53As interfaces. <i>Physical Review B</i> , <b>1990</b> , 41, 12106-12110  | 3.3 | 38   |
| 12 | Theory of band offsets at semiconductor heterojunctions: An ab-initio linear response approach. <i>Superlattices and Microstructures</i> , <b>1989</b> , 6, 31-37                  | 2.8 | 21   |
| 11 | Theoretical study of cubic versus tetragonal structures of defect zinc-blende semiconductors: CdIn2Se4. <i>Physical Review B</i> , <b>1989</b> , 40, 1725-1731                     | 3.3 | 23   |
| 10 | Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. <i>Physical Review Letters</i> , <b>1989</b> , 62, 2853-2856                        | 7.4 | 161  |
| 9  | Band offsets in lattice-matched heterojunctions: A model and first-principles calculations for GaAs/AlAs. <i>Physical Review Letters</i> , <b>1988</b> , 61, 734-737               | 7.4 | 465  |
| 8  | Structural and electronic properties of spinel semiconductors: An ab initio pseudopotential study of MgIn2S. <i>Physical Review B</i> , <b>1988</b> , 38, 8258-8263                | 3.3 | 26   |
| 7  | Pressure-induced structural instability of cesium halides from ab initio pseudopotential techniques. <i>Physical Review B</i> , <b>1987</b> , 35, 765-769                          | 3.3 | 12   |
| 6  | Elastic constants of crystals from linear-response theory. <i>Physical Review Letters</i> , <b>1987</b> , 59, 2662-2665  | 7.4 | 73   |
| 5  | Green's-function approach to linear response in solids. <i>Physical Review Letters</i> , <b>1987</b> , 58, 1861-1864   | 7.4 | 1546 |
| 4  | Ab initio calculation of the macroscopic dielectric constant in silicon. <i>Physical Review B</i> , <b>1986</b> , 33, 7017-7021  | 3.3 | 406  |
| 3  | Exact-exchange extension of the local-spin-density approximation in atoms. II. The iron series. <i>Journal of Chemical Physics</i> , <b>1984</b> , 80, 5703-5708                   | 3.9 | 26   |
| 2  | Hartree-Fock energy bands in molecular crystals: Solid hydrogen in the cubic phase. <i>Physical Review B</i> , <b>1984</b> , 30, 7187-7193   | 3.3 | 7    |

- 1 Exact-exchange extension of the local-spin-density approximation in atoms: Calculation of total energies and electron affinities. *Journal of Chemical Physics*, **1983**, 79, 6140-6144 3.9 60