

Francesco Sebastianelli

List of Publications by Year in descending order

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37
papers

1,024
citations

394421

19
h-index

414414

32
g-index

39
all docs

39
docs citations

39
times ranked

569
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Hydrogen Molecule in the Small Dodecahedral Cage of a Clathrate Hydrate: Quantum Five-Dimensional Calculations of the Coupled Translation-Rotation Eigenstates. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24806-24811. | 2.6 | 83 |
| 2 | H ₂ , HD, and D ₂ inside C ₆₀ : Coupled translation-rotation eigenstates of the endohedral molecules from quantum five-dimensional calculations. <i>Journal of Chemical Physics</i> , 2008, 129, 064313. | 3.0 | 80 |
| 3 | Quantum dynamics of coupled translational and rotational motions of H ₂ inside C ₆₀ . <i>Journal of Chemical Physics</i> , 2008, 128, 011101. | 3.0 | 74 |
| 4 | Coupled translation-rotation eigenstates of H ₂ in C ₆₀ and C ₇₀ on the spectroscopically optimized interaction potential: Effects of cage anisotropy on the energy level structure and assignments. <i>Journal of Chemical Physics</i> , 2009, 130, 224306. | 3.0 | 69 |
| 5 | Quantum dynamics of H ₂ , D ₂ , and HD in the small dodecahedral cage of clathrate hydrate: Evaluating H ₂ -water nanocage interaction potentials by comparison of theory with inelastic neutron scattering experiments. <i>Journal of Chemical Physics</i> , 2008, 128, 244715. | 3.0 | 66 |
| 6 | Quantum dynamics of small H ₂ and D ₂ clusters in the large cage of structure II clathrate hydrate: Energetics, occupancy, and vibrationally averaged cluster structures. <i>Journal of Chemical Physics</i> , 2008, 129, 244706. | 3.0 | 59 |
| 7 | Hydrogen Molecules inside Fullerene C ₇₀ : Quantum Dynamics, Energetics, Maximum Occupancy, And Comparison with C ₆₀ . <i>Journal of the American Chemical Society</i> , 2010, 132, 9826-9832. | 13.7 | 51 |
| 8 | Path Integral Molecular Dynamics Study of Small H ₂ Clusters in the Large Cage of Structure II Clathrate Hydrate: Temperature Dependence of Quantum Spatial Distributions. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20775-20782. | 3.1 | 48 |
| 9 | Hydrogen Molecules in the Small Dodecahedral Cage of a Clathrate Hydrate: Quantum Translation-Rotation Dynamics of the Confined Molecules. <i>Journal of Physical Chemistry C</i> , 2007, 111, 2497-2504. | 3.1 | 45 |
| 10 | Coupled Translation-Rotation Eigenstates of H ₂ , HD, and D ₂ in the Large Cage of Structure II Clathrate Hydrate: Comparison with the Small Cage and Rotational Raman Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7601-7609. | 2.5 | 41 |
| 11 | Dissociative Electron Attachment to Formamide: Direct and Indirect Pathways from Resonant Intermediates. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 217-221. | 5.3 | 34 |
| 12 | Electron scattering cross sections from HCN over a broad energy range (0.1–10 ⁴ eV): Influence of the permanent dipole moment on the scattering process. <i>Journal of Chemical Physics</i> , 2012, 137, 124103. | 3.0 | 34 |
| 13 | Microsolvation of Li ⁺ in Small He Clusters. Li ⁺ He _n Species from Classical and Quantum Calculations. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1045-1054. | 5.3 | 32 |
| 14 | Hydrogen Molecule in the Small Dodecahedral Cage of a Clathrate Hydrate: Quantum Translation-Rotation Dynamics at Higher Excitation Energies. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12763-12771. | 2.5 | 30 |
| 15 | One and Two Hydrogen Molecules in the Large Cage of the Structure II Clathrate Hydrate: Quantum Translation-Rotation Dynamics Close to the Cage Wall. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6115-6121. | 2.5 | 27 |
| 16 | Ab initio quantum dynamics with very weak van der Waals interactions: Structure and stability of small Li ₂ (He) _n clusters. <i>Journal of Chemical Physics</i> , 2004, 120, 9160-9166. | 3.0 | 25 |
| 17 | Quantum and classical structures for 4He clusters with the H ⁺ impurity. <i>Journal of Chemical Physics</i> , 2003, 119, 8276-8288. | 3.0 | 22 |
| 18 | Microsolvation of Li ⁺ in bosonic helium clusters. I. Many-body effects on the structures of the small aggregates. <i>Computational Materials Science</i> , 2006, 35, 261-267. | 3.0 | 21 |

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|----|--|-----|-----------|
| 19 | Structural and quantum effects from anionic centers in rare gas clusters: The $(\text{Ne})_n\text{H}^-$ and $(\text{Ne})_{n+1}$ systems. <i>Journal of Chemical Physics</i> , 2003, 119, 5570-5582. | 3.0 | 20 |
| 20 | Gas-phase route to polycyclic aromatic hydrocarbon formation in protoplanetary atmospheres: role of stabilized benzyne anions. <i>Monthly Notices of the Royal Astronomical Society</i> , 2011, 415, 425-430. | 4.4 | 16 |
| 21 | ELECTRON-DRIVEN REACTIONS IN PROTO-PLANETARY ATMOSPHERES: METASTABLE ANIONS OF GASEOUS o-BENZYNE. <i>Astrophysical Journal</i> , 2010, 712, 445-452. | 4.5 | 15 |
| 22 | Forming $(\text{NCCN})^-$ by quantum scattering: A modeling for Titan's atmosphere. <i>Chemical Physics</i> , 2012, 398, 199-205. | 1.9 | 14 |
| 23 | Rotational cooling of $\text{Li}_2(1^2g^+)$ molecules by ultracold collisions with a helium gas buffer. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 263. | 1.4 | 13 |
| 24 | Modelling ionic nucleation in small neon clusters. <i>International Journal of Mass Spectrometry</i> , 2002, 220, 193-209. | 1.5 | 12 |
| 25 | Microsolvation of LiH in Helium Clusters: Many-Body Effects and Additivity Models for the Interaction Forces. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4252-4260. | 2.5 | 12 |
| 26 | HF in clusters of molecular hydrogen: II. Quantum solvation by H_2 isotopomers, cluster rigidity, and comparison with CO-doped parahydrogen clusters. <i>Journal of Chemical Physics</i> , 2006, 125, 164313. | 3.0 | 10 |
| 27 | | | |

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|----|---|-----|-----------|
| 37 | Scattering of electrons by gaseous CS(1 $\hat{\Sigma}$): The role of short-range forces on the very-low energy 2 $\hat{\Sigma}$ resonance. Chemical Physics Letters, 2009, 476, 182-185. | 2.6 | 2 |