

Johnatan Mucelini

List of Publications by Year in descending order

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Version: 2024-02-01

8
papers

106
citations

1684188
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88
citing authors

| # | ARTICLE | IF | CITATIONS |
|---|---|-----|-----------|
| 1 | Machine Learning Prediction of Nine Molecular Properties Based on the SMILES Representation of the QM9 Quantum-Chemistry Dataset. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9854-9866. | 2.5 | 50 |
| 2 | <i>Ab Initio</i> Insights into the Formation Mechanisms of 55-Atom Pt-Based Core-Shell Nanoalloys. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1158-1164. | 3.1 | 22 |
| 3 | Methane dehydrogenation on 3d 13-atom transition-metal clusters: A density functional theory investigation combined with Spearman rank correlation analysis. <i>Fuel</i> , 2020, 275, 117790. | 6.4 | 14 |
| 4 | <i>Ab initio</i> investigation of the formation of ZrO ₂ -like structures upon the adsorption of Zr on the CeO ₂ (111) surface. <i>Journal of Chemical Physics</i> , 2018, 149, 244702. | 3.0 | 7 |
| 5 | Understanding the interplay between π - π and cation- π interactions in [Janusene- ⁺ Ag] ⁺ guest systems: a computational approach. <i>Dalton Transactions</i> , 2019, 48, 13281-13292. | 3.3 | 7 |
| 6 | Ab initio insights into the structural, energetic, electronic, and stability properties of mixed CeZr ₁₅ N ₃₀ nanoclusters. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26637-26646. | 2.8 | 3 |
| 7 | Correlation-Based Framework for Extraction of Insights from Quantum Chemistry Databases: Applications for Nanoclusters. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1125-1135. | 5.4 | 3 |
| 8 | From Bulk CeO ₂ to Transition-Metal Clusters Supported on the CeO ₂ (111) Surface: A Critical Discussion. , 2018, , 452-459. | | 0 |