# Quan-De Wang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4282636/publications.pdf

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|---|---|---|---|
| 63 papers | 1,241 citations | 489802 18 h-index | 445137 33 g-index |
| 64 all docs | 64 docs citations | 64 times ranked | 1371 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | A comparative single-pulse shock tube experiment and kinetic modeling study on pyrolysis of cyclohexane, methylcyclohexane and ethylcyclohexane. Defence Technology, 2023, 20, 137-148. | 2.1 | 7 |
| 2 | Experimental study on sooting characteristics of a direct coal liquefaction derived jet fuel and its blend with RP-3 jet fuel. Fuel, 2022, 307, 121846. | 3.4 | 8 |
| 3 | A Hierarchical Theoretical Study of the Hydrogen Abstraction Reactions of H<sub>2</sub>/C<sub>1</sub>â€“C<sub>4</sub> Molecules by the Methyl Peroxy Radical and Implications for Kinetic Modeling. ACS Omega, 2022, 7, 8675-8685. | 1.6 | 2 |
| 4 | Simultaneous measurements of temperature, CO, and CO2 time-history in reacting n-heptane/O2/argon mixtures blended with diethyl ether behind reflected shock waves. Combustion and Flame, 2022, 241, 112057. | 2.8 | 11 |
| 5 | Comparative study on ignition characteristics of n-propylbenzene, 1,3,5-trimethylbenzene and 1,2,4-trimethylbenzene behind reflected shock waves. Fuel, 2022, 325, 124940. | 3.4 | 11 |
| 6 | Development of machine learning models for the prediction of laminar flame speeds of hydrocarbon and oxygenated fuels. Fuel Communications, 2022, 12, 100071. | 2.0 | 7 |
| 7 | Development of a 5-component gasoline surrogate model using recent advancements in the detailed H2/O2/CO/C1-C3 mechanism for decoupling methodology. Fuel, 2021, 283, 118793. | 3.4 | 12 |
| 8 | Theoretical study of the hydrogen abstraction reactions from substituted phenolic species. Computational and Theoretical Chemistry, 2021, 1196, 113120. | 1.1 | 6 |
| 9 | Accurate prediction of standard enthalpy of formation based on semiempirical quantum chemistry methods with artificial neural network and molecular descriptors. International Journal of Quantum Chemistry, 2021, 121, e26441. | 1.0 | 13 |
| 10 | Benchmark calculations for bond dissociation energies and enthalpy of formation of chlorinated and brominated polycyclic aromatic hydrocarbons. RSC Advances, 2021, 11, 29690-29701. | 1.7 | 5 |
| 11 | Prediction of band gap for 2D hybrid organicâ€“inorganic perovskites by using machine learning through molecular graphics descriptors. New Journal of Chemistry, 2021, 45, 9427-9433. | 1.4 | 11 |
| 12 | Data-driven machine learning model for the prediction of oxygen vacancy formation energy of metal oxide materials. Physical Chemistry Chemical Physics, 2021, 23, 15675-15684. | 1.3 | 8 |
| 13 | Development of Multipurpose Skeletal Core Combustion Chemical Kinetic Mechanisms. Energy & Fuels, 2021, 35, 6921-6927. | 2.5 | 18 |
| 14 | Single-Pulse Shock Tube Pyrolysis Study of RP-3 Jet Fuel and Kinetic Modeling. ACS Omega, 2021, 6, 11039-11047. | 1.6 | 16 |
| 15 | Ignition characteristics of an alternative kerosene from direct coal liquefaction and its blends with conventional RP-3 jet fuel. Fuel, 2021, 291, 120258. | 3.4 | 23 |
| 16 | Machine learning prediction of the optimal carrier concentration and band gap of quaternary thermoelectric materials via element feature descriptors. International Journal of Quantum Chemistry, 2021, 121, e26752. | 1.0 | 4 |
| 17 | Discovery of ester lubricants with low coefficient of friction on material surface via machine learning. Chemical Physics Letters, 2021, 773, 138589. | 1.2 | 12 |
| 18 | Single-Pulse Shock Tube Experimental and Kinetic Modeling Study on Pyrolysis of a Direct Coal Liquefaction-Derived Jet Fuel and Its Blends with the Traditional RP-3 Jet Fuel. ACS Omega, 2021, 6, 18442-18450. | 1.6 | 10 |

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|---|---|---|---|
| 19 | Machine learning prediction of stability, topological properties and band gap of topological insulators in tetradymites. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 409, 127508. | 0.9 | 0 |
| 20 | Effectively improving the accuracy of PBE functional in calculating the solid band gap via machine learning. Computational Materials Science, 2021, 198, 110699. | 1.4 | 25 |
| 21 | An experimental and detailed kinetic modeling study of the pyrolysis and oxidation of allene and propyne over a wide range of conditions. Combustion and Flame, 2021, 233, 111578. | 2.8 | 26 |
| 22 | Accelerating the optimization of enzyme-catalyzed synthesis conditions via machine learning and reactivity descriptors. Organic and Biomolecular Chemistry, 2021, 19, 6267-6273. | 1.5 | 5 |
| 23 | Machine Learning Prediction of the Exfoliation Energies of Two-Dimension Materials via Data-Driven Approach. Journal of Physical Chemistry Letters, 2021, 12, 11470-11475. | 2.1 | 7 |
| 24 | Active P species in P-doped graphite carriers improving the electrocatalytic performance of supported Pt towards the hydrogen evolution reaction. New Journal of Chemistry, 2021, 45, 21670-21675. | 1.4 | 4 |
| 25 | Comparative Chemical Kinetic Analysis and Skeletal Mechanism Generation for Syngas Combustion with NO<sub>x</sub> Chemistry. Energy & Fuels, 2020, 34, 949-964. | 2.5 | 19 |
| 26 | Hindered rotor benchmarks for the transition states of free radical additions to unsaturated hydrocarbons. Physical Chemistry Chemical Physics, 2020, 22, 27241-27254. | 1.3 | 2 |
| 27 | Evaluation of non-ideal piston stopping effects on the â€œadiabatic coreâ€•and ignition delay time simulation in rapid compression machines. Combustion and Flame, 2020, 218, 229-233. | 2.8 | 3 |
| 28 | Skeletal chemical kinetic mechanism generation for methanol combustion and systematic analysis on the ignition characteristics. Asia-Pacific Journal of Chemical Engineering, 2020, 15, e2434. | 0.8 | 6 |
| 29 | Phosphorousâ€Doped Graphite Layers with Outstanding Electrocatalytic Activities for the Oxygen and Hydrogen Evolution Reactions in Water Electrolysis. Advanced Functional Materials, 2020, 30, 1910741. | 7.8 | 48 |
| 30 | Accurate prediction of enthalpy of formation combined with AM1 method and molecular descriptors. Chemical Physics Letters, 2020, 747, 137327. | 1.2 | 3 |
| 31 | An approach to avoid the mix potential for Pt-based cathode catalysts in the direct ethanol fuel cell. Materials Letters, 2020, 274, 128002. | 1.3 | 2 |
| 32 | Influences of N species in N-doped carbon carriers on the catalytic performance of supported Pt. Materials Chemistry and Physics, 2019, 237, 121881. | 2.0 | 10 |
| 33 | Chemical Kinetics of Hydrogen Atom Abstraction from Propargyl Sites by Hydrogen and Hydroxy Radicals. International Journal of Molecular Sciences, 2019, 20, 3227. | 1.8 | 6 |
| 34 | High-level theoretical study of the hydrogen abstraction reaction H2Sâ€¯+â€¯O2â€¯=â€¯SHâ€¯+â€¯HO2 and prediction of the rate constants. Computational and Theoretical Chemistry, 2019, 1155, 61-66. | 1.1 | 3 |
| 35 | Reaction Mechanisms and Kinetics of the Hydrogen Abstraction Reactions of C4â€“C6 Alkenes with Hydroxyl Radical: A Theoretical Exploration. International Journal of Molecular Sciences, 2019, 20, 1275. | 1.8 | 19 |
| 36 | The identification of activeÂN species in N-doped carbon carriers that improve the activity of Fe electrocatalysts towards the oxygen evolution reaction. RSC Advances, 2019, 9, 4806-4811. | 1.7 | 7 |

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|---|---|---|---|
| 37 | Reaction Kinetics of Hydrogen Atom Abstraction from C4â€“C6 Alkenes by the Hydrogen Atom and Methyl Radical. Journal of Physical Chemistry A, 2018, 122, 5202-5210. | 1.1 | 15 |
| 38 | Theoretical studies of unimolecular thermal decomposition reactions of n -hexane and n -hexene isomers. Computational and Theoretical Chemistry, 2017, 1115, 45-55. | 1.1 | 11 |
| 39 | Theoretical studies on the hydrogen abstraction reactions of methyl esters with HO<sub>2</sub>radical and the following Î²-scission reactions. Journal of Physical Organic Chemistry, 2017, 30, e3668. | 0.9 | 10 |
| 40 | Germanium-doped and germanium/nitrogen-codoped carbon nanotubes with highly enhanced activity for oxygen reduction in alkaline medium. RSC Advances, 2016, 6, 72676-72680. | 1.7 | 6 |
| 41 | Theoretical and kinetic study of the hydrogen atom abstraction reactions of unsaturated C6 methyl esters with hydroxyl radical. Chemical Physics Letters, 2016, 650, 119-125. | 1.2 | 18 |
| 42 | Novel As-doped, As and N-codoped carbon nanotubes as highly active and durable electrocatalysts for O2 reduction in alkaline medium. Journal of Power Sources, 2016, 306, 535-540. | 4.0 | 18 |
| 43 | Skeletal Mechanism Generation for Methyl Butanoate Combustion via Directed Relation Graph Based Methods. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2016, 32, 595-604. | 2.2 | 9 |
| 44 | Si-doped carbon nanotubes as efficient metal-free electrocatalysts for O2 reduction in alkaline medium. Materials Letters, 2015, 158, 32-35. | 1.3 | 27 |
| 45 | Novel silicon-doped, silicon and nitrogen-codoped carbon nanomaterials with high activity for the oxygen reduction reaction in alkaline medium. Journal of Materials Chemistry A, 2015, 3, 3289-3293. | 5.2 | 77 |
| 46 | Influence of the double bond on the hydrogen abstraction reactions of methyl esters with hydrogen radical: an ab initio and chemical kinetic study. RSC Advances, 2015, 5, 68314-68325. | 1.7 | 23 |
| 47 | Low Pt content catalyst supported on nitrogen and phosphorus-codoped carbon nanotubes for electrocatalytic O2 reaction in acidic medium. Materials Letters, 2015, 142, 115-118. | 1.3 | 15 |
| 48 | Phosphorus-doped carbon nanotubes supported low Pt loading catalyst for the oxygen reduction reaction in acidic fuel cells. Journal of Power Sources, 2014, 268, 171-175. | 4.0 | 61 |
| 49 | An updated detailed reaction mechanism for syngas combustion. RSC Advances, 2014, 4, 4564-4585. | 1.7 | 8 |
| 50 | An application of the reaction class transition state theory to the kinetics of hydrogen abstraction reactions of hydrogen with methyl esters at the methoxy group. Computational and Theoretical Chemistry, 2014, 1027, 103-111. | 1.1 | 24 |
| 51 | Theoretical and kinetic study of the hydrogen atom abstraction reactions of ethyl esters with hydrogen radicals. Chemical Physics Letters, 2014, 616-617, 109-114. | 1.2 | 28 |
| 52 | Skeletal Mechanism Generation for High-Temperature Combustion of H<sub>2</sub>/CO/C<sub>1</sub>â€“C<sub>4</sub> Hydrocarbons. Energy & Fuels, 2013, 27, 4021-4030. | 2.5 | 31 |
| 53 | Systematic analysis and reduction of combustion mechanisms for ignition of multi-component kerosene surrogate. Proceedings of the Combustion Institute, 2013, 34, 187-195. | 2.4 | 36 |
| 54 | ReaxFF Molecular Dynamics Simulations of Oxidation of Toluene at High Temperatures. Journal of Physical Chemistry A, 2012, 116, 9811-9818. | 1.1 | 117 |

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|---|---|---|---|
| 55 | Effects of Fuel Additives on the Thermal Cracking of n-Decane from Reactive Molecular Dynamics. Journal of Physical Chemistry A, 2012, 116, 3794-3801. | 1.1 | 37 |
| 56 | Skeletal mechanism generation for high-temperature oxidation of kerosene surrogates. Combustion and Flame, 2012, 159, 91-102. | 2.8 | 32 |
| 57 | Reduction of the Detailed Kinetic Mechanism for High-Temperature Combustion of <em>n</em>-Dodecane. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2012, 28, 2536-2542. | 2.2 | 5 |
| 58 | Computational Study of the Reaction Mechanism of the Methylperoxy Self-Reaction. Journal of Physical Chemistry A, 2011, 115, 13534-13541. | 1.1 | 33 |
| 59 | Reactive molecular dynamics simulation and chemical kinetic modeling of pyrolysis and combustion of n-dodecane. Combustion and Flame, 2011, 158, 217-226. | 2.8 | 196 |
| 60 | Mechanism Construction and Simulation for the High-Temperature Combustion of <em>n</em>-Dodecane. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2011, 27, 2755-2761. | 2.2 | 6 |
| 61 | Time-Dependent Stokes Shift from Solvent Dielectric Relaxation. Chinese Journal of Chemical Physics, 2010, 23, 297-302. | 0.6 | 1 |
| 62 | Nonequilibrium solvation energy by means of constrained equilibrium thermodynamics and its application to self-exchange electron transfer reactions. Physical Chemistry Chemical Physics, 2010, 12, 1341-1350. | 1.3 | 17 |
| 63 | Continuum Model for Electronic Polarization Based on a Novel Dielectric Response Function. Chinese Journal of Chemical Physics, 2009, 22, 481-488. | 0.6 | 1 |