

# Publications intéressantes

## Dans Journal of Chemical Education

### 2023

- [Foregrounding the Code: Computational Chemistry Instructional Activities Using a Highly Readable Fluid Simulation Code](#)
- [An Alternative Experimental Procedure to Determine the Solubility of Potassium Nitrate in Water with Automatic Data Acquisition Using Arduino for Secondary School: Development and Validation with Pre-Service Chemistry Teachers](#)
- [A Computational Experiment Introducing Undergraduates to Geometry Optimizations, Vibrational Frequencies, and Potential Energy Surfaces](#)
- [Interactive Python Notebooks for Physical Chemistry](#)
- [Interactive Learning of Diffusion and the Diffusion Equation with Mathematical Software | Journal of Chemical Education](#)

### 2021



- [Applying Density Functional Theory to Common Organic Mechanisms: A Computational Exercise](#)  
Jonathan P. Antle, Masashi W. Kimura, Stefano Racioppi, Corey Damon, Meredith Lang, Caitlyn Gatley-Montross, Laura S. Sánchez B., Daniel P. Miller, Eva Zurek, Adam M. Brown, Kellie Gast, and Scott M. Simpson, J. Chem. Educ. 2022, XXXX, XXX, XXX-XXX Publication  
Date: November 30, 2022 DOI: 10.1021/acs.jchemed.2c00935

### 2021



### 2020



### 2019

- [Total Chemical Footprint of an Experiment: A Systems Thinking Approach to Teaching Rovibrational Spectroscopy](#)  
Paul D. Cooper, Jacob Walser, J. Chem. Educ. 2019, 96(12), 2947-2951 DOI: 10.1021/acs.jchemed.9b00405

- [Valorization of Waste Orange Peel to Produce Shear-Thinning Gels](#) Lucy S. Mackenzie, Helen Tyrrell, Robert Thomas, Avtar S. Matharu, James H. Clark, Glenn A. Hurst, *J. Chem. Educ.* 2019, 96(12), 3025-3029 DOI: 10.1021/acs.jchemed.8b01009
- [Helping Students Connect Interdisciplinary Concepts and Skills in Physical Chemistry and Introductory Computing: Solving Schrödinger's Equation for the Hydrogen Atom](#) Oka Kurniawan, Li Ling Apple Koh, Jermaine Zhi Min Cheng, Maggie Pee, *J. Chem. Educ.* 2019, 96(10), 2202-2207 DOI: 10.1021/acs.jchemed.9b00068
- [Teaching Entropy from Phase Space Perspective: Connecting the Statistical and Thermodynamic Views Using a Simple One-Dimensional Model](#) Dhritiman Bhattacharyya, Jahan M. Dawlaty, *J. Chem. Educ.* 2019, 96(10), 2208-2216 DOI: 10.1021/acs.jchemed.9b00134
- [Demystifying Mathematical Modeling of Electrochemical Systems](#) Lisa I. Stephens, Janine Mauzeroll, *J. Chem. Educ.* 2019, 96(10), 2217-2224 DOI: 10.1021/acs.jchemed.9b00542
- [Development of the Enthalpy and Entropy in Dissolution and Precipitation Inventory](#) Timothy N. Abell, Stacey Lowery Bretz, *J. Chem. Educ.* 2019, 96(9), 1804-1812, DOI: 10.1021/acs.jchemed.9b00186
- [Investigating Student Understanding of London Dispersion Forces: A Longitudinal Study](#) Keenan Noyes, Melanie M. Cooper, *J. Chem. Educ.* 2019, 96(9), 1821-1832 DOI: 10.1021/acs.jchemed.9b00455
- [Bouncing Droplets: A Hands-On Activity To Demonstrate the Properties and Applications of Superhydrophobic Surface Coatings](#) Carolina Cionti, Tommaso Taroni, Daniela Meroni, *J. Chem. Educ.* 2019, 96(9), 1971-1976 DOI: 10.1021/acs.jchemed.9b00406
- [Chemical Curiosity on Campus: An Undergraduate Project on the Structure and Wettability of Natural Surfaces](#) Anthony Katselas, Alice Motion, Chiara O'Reilly, Chiara Neto, *J. Chem. Educ.* 2019, 96(9), 1998-2002 DOI: 10.1021/acs.jchemed.9b00324
- [Alternative Derivation of the Maxwell Distribution of Speeds](#) Francisco Rivadulla, *J. Chem. Educ.* 2019, 96(9), 2063-2065 DOI: 10.1021/acs.jchemed.9b00188
- [Realistic Implementation of the Particle Model for the Visualization of Nanoparticle Precipitation and Growth](#) Antonella Di Vincenzo, Michele A. Floriano, *J. Chem. Educ.* 2019, 96(8), 1654-1662 DOI: 10.1021/acs.jchemed.9b00330
- [Implementing New Educational Platforms in the Classroom: An Interactive Approach to the Particle in a Box Problem](#) Vinícius Wilian D. Cruzeiro, Xiang Gao, Valeria D. Kleiman, *J. Chem. Educ.* 2019, 96(8), 1663-1670 DOI: 10.1021/acs.jchemed.9b00195
- [Development of the Quantization and Probability Representations Inventory as a Measure of Students' Understandings of Particulate and Symbolic Representations of Electron Structure](#) Zahilyn D. Roche Allred, Stacey Lowery Bretz, *J. Chem. Educ.* 2019, 96(8), 1558-1570 DOI: 10.1021/acs.jchemed.9b00098
- [Developing and Using a Computer Simulation of Liquid-Vapor Transitions to Improve Students' Assimilation of Concepts Related to the Behavior of Real Gases](#) David Zorrilla, Jesús Sánchez-Márquez, Víctor García, Manuel Fernández, *J. Chem. Educ.* 2019, 96(8), 1646-1653 DOI: 10.1021/acs.jchemed.8b00939
- [Enthalpy and the Second Law of Thermodynamics](#) David Keifer, *J. Chem. Educ.*, 2019, 96 (7), pp 1407-1411 DOI: 10.1021/acs.jchemed.9b00326
- [µdroPi: A Hand-Held Microfluidic Droplet Imager and Analyzer Built on Raspberry Pi](#) Meng Sun, Zhengda LiQiong Yang, *J. Chem. Educ.*, 2019, 96 (6), pp 1152-1156 DOI: 10.1021/acs.jchemed.8b00975
- [PChem Challenge Game: Reinforcing Learning in Physical Chemistry](#) Tugba G. Kucukkal, Ajda Kahveci, *J. Chem. Educ.*, 2019, 96 (6), pp 1187-1193 DOI: 10.1021/acs.jchemed.8b00757
- [Effect of Chemical and Physical Modifications on the Wettability of Polydimethylsiloxane Surfaces](#) Carolyn L. Wanamaker, Brittany S. Neff, Azieta Nejati-Namin, Erin R. Spatenka, Mong-Lin Yang, *J. Chem. Educ.*, 2019, 96 (6), pp 1212-1217 DOI: 10.1021/acs.jchemed.8b00814
- [Disseminating a Free, Practical Java Tool To Interactively Generate and Edit 2D Chemical](#)

- [Structures](#) Andreas Hofmann, Mark J. Coster, Paul Taylor, J. Chem. Educ., 2019, 96 (6), pp 1262-1267 DOI: 10.1021/acs.jchemed.9b00073
- [Design, Fabrication, and Optical Characterization of a Low-Cost and Open-Source Spin Coater](#) Mohammad Sadegh-cheri, J. Chem. Educ., 2019, 96 (6), pp 1268-1272 DOI: 10.1021/acs.jchemed.9b00013
  - [Collaborative Learning Exercises for Teaching Protein Mass Spectrometry](#) Michelle L. Kovarik, Jill K. Robinson, J. Chem. Educ. 2019, 96 (5) pp905-911 DOI: 10.1021/acs.jchemed.8b00734 + [Biological Mass Spectrometry: Proteomics](#)
  - [A Tale of Two Molecules: How the Heat Capacities of N<sub>2</sub>\(g\) and F<sub>2</sub>\(g\) Differ At High Temperature and Why Naïve Expectations Fail to Explain These Differences: A Spreadsheet Exercise for Physical Chemistry Students](#) Arthur M. Halpern and Robert J. Noll, J. Chem. Educ., 2019, 96 (5), pp 926-935 DOI: 10.1021/acs.jchemed.9b00029
  - [Creating and Experimenting with a Low-Cost, Rugged System to Visually Demonstrate the Vapor Pressure of Liquids as a Function of Temperature](#) Rodrigo Papai, Mayara Araujo Romano, Aline Rodrigues Arroyo, Bárbara Rodrigues da Silva, Bruno Tresoldi, Gabriela Cabo Winter, Julia Messias Costa, Maria Aparecida Freitas Santos, Matheus Damasceno Prata, and Ivanise Gaubeur, J. Chem. Educ., 2019, 96 (2), pp 335-341 DOI: 10.1021/acs.jchemed.8b00381
  - [Teaching Boyle's Law and Charles' Law through Experiments that Use Novel, Inexpensive Equipment Yielding Accurate Results](#) Taweetham Limpanuparb, Siradanai Kanithasevi, Maytouch Lojanarungsiri, and Puh Pakwilaikiat, J. Chem. Educ., 2019, 96 (1), pp 169-174 DOI: 10.1021/acs.jchemed.8b00460
  - [Simple and Low-Cost Setup for Measurement of the Density of a Liquid](#) Nima Noei, Iman Mohammadi Imani, Lee D. Wilson, and Saeid Azizian, J. Chem. Educ., 2019, 96 (1), pp 175-179 DOI: 10.1021/acs.jchemed.7b00979
  - [Reduction of Water Waste in an Organic Chemistry Laboratory Using a Low-Cost Recirculation System for Condenser Apparatus](#) Alex Schoeddert, Keshwaree Babooram, and Sarah Pelletier J. Chem. Educ., 2019, 96 (1), pp 180-182 DOI: 10.1021/acs.jchemed.8b00400
  - [Graphical Representation of Hydrogenic Orbitals: Incorporating Both Radial and Angular Parts of the Wave Function](#) Meghna A. Manae and Anirban Hazra, J. Chem. Educ., 2019, 96 (1), pp 187-190 DOI: 10.1021/acs.jchemed.8b00372

## 2018

- [Wetting Modification by Photocatalysis: A Hands-on Activity To Demonstrate Photoactivated Reactions at Semiconductor Surfaces](#) Luca Rimoldi, Tommaso Taroni, and Daniela Meroni, J. Chem. Educ., 2018, 95 (12), pp 2216-2221 DOI: 10.1021/acs.jchemed.8b00362
- [Constructing the Phase Diagram of a Single-Component System Using Fundamental Principles of Thermodynamics and Statistical Mechanics: A Spreadsheet-Based Learning Experience for Students](#) Arthur M. Halpern and Charles J. Marzzacco, J. Chem. Educ., 2018, 95 (12), pp 2197-2204 DOI: 10.1021/acs.jchemed.8b00560
- [Using the Principles of Classical and Statistical Thermodynamics To Calculate the Melting and Boiling Points, Enthalpies and Entropies of Fusion and Vaporization of Water, and the Freezing Point Depression and Boiling Point Elevation of Ideal and Nonideal Aqueous Solutions](#) Arthur M. Halpern and Charles J. Marzzacco, J. Chem. Educ., 2018, 95 (12), pp 2205-2211 DOI: 10.1021/acs.jchemed.8b00561
- [The Gibbs Phase Rule: What Happens When Some Phases Lack Some Components?](#) Deepika Janakiraman, J. Chem. Educ., 2018, 95 (11), pp 2086-2088 DOI: 10.1021/acs.jchemed.8b00377
- [Liquid Crystal Demonstration of Binary Phase Behavior for the Classroom](#) Marissa E. Tousley, J. Chem. Educ., 2018, 95 (11), pp 2000-2005 DOI: 10.1021/acs.jchemed.8b00081
- [Approximate Equation To Calculate Partial Pressures in a Mixture of Real Gases](#) Bernard Hayez,

- J. Chem. Educ., 2018, 95 (11), pp 1982–1988 DOI: 10.1021/acs.jchemed.8b00185
- [Investigation of the Ternary Phase Diagram of Water–Propan-2-ol–Sodium Chloride: A Laboratory Experiment](#) Cory C. Pye, M. Angelique Imperial, Coltin Elson, Megan L. Himmelman, Jacquelyn A. White, and Fuhao Lin, J. Chem. Educ., 2018, 95 (8), pp 1398–1401 DOI: 10.1021/acs.jchemed.8b00242
  - [Pedagogical Approach to the Modeling and Simulation of Oscillating Chemical Systems with Modern Software: The Brusselator Model](#) Jaime H. Lozano-Parada, Helen Burnham, and Fiderman Machuca Martinez, J. Chem. Educ., 2018, 95 (5), pp 758–766 DOI: 10.1021/acs.jchemed.7b00703
  - [Facilitating Students' Interaction with Real Gas Properties Using a Discovery-Based Approach and Molecular Dynamics Simulations](#) Chelsea Sweet, Oyewumi Akinfenwa, and Jonathan J. Foley, IV J. Chem. Educ., 2018, 95 (3), pp 384–392 DOI: 10.1021/acs.jchemed.7b00747

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- [Development and Use of an Open-Source, User-Friendly Package To Simulate Voltammetry Experiments](#) Shuo Wang, Jing Wang, and Yanjing Gao, J. Chem. Educ., 2017, 94 (10), pp 1567–1570 DOI: 10.1021/acs.jchemed.6b00986
- [Adapting and Modifying the Apparatus for Students To Accurately Determine the Freezing Point of a Solvent and Solution](#) Shirong Li, Jianzhong Guo, Kewang Wang, Lin Chen, Daodao Hu, and Yunshan Bai, J. Chem. Educ., 2017, 94 (10), pp 1590–1593 DOI: 10.1021/acs.jchemed.7b00253
- [Periodic Reactions: The Early Works of William C. Bray and Alfred J. Lotka](#) Rinaldo Cervellati and Emanuela Greco, J. Chem. Educ., 2017, 94 (2), pp 195–201 DOI: 10.1021/acs.jchemed.6b00342
- [Partially Miscible Water–Triethylamine Solutions and Their Temperature Dependence](#), Johan P. Erikson, J. Chem. Educ., 2017, 94 (1), pp 75–78 DOI: 10.1021/acs.jchemed.6b00489

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- [From Discrete to Continuous Process Simulation in Classical Thermodynamics: Irreversible Expansions of Ideal Monatomic Gases](#), Carmen Álvarez-Rúa, Javier Borge, J. Chem. Educ., 2016, 93 (12), pp 2110–2116 DOI: 10.1021/acs.jchemed.6b00226
  - correction : <http://pubs.acs.org/doi/abs/10.1021/acs.jchemed.7b00132>
- [Improving Students' Understanding of the Connections between the Concepts of Real-Gas Mixtures, Gas Ideal-Solutions, and Perfect-Gas Mixtures](#), Romain Privat, Jean-Noël Jaubert, and Edouard Moine, J. Chem. Educ., 2016, 93 (12), pp 2040–2045 DOI: 10.1021/acs.jchemed.6b00553
- [Let Students Derive, by Themselves, Two-Dimensional Atomic and Molecular Quantum Chemistry from Scratch](#), Yingbin Ge, J. Chem. Educ., 2016, 93 (12), pp 2033–2039 DOI: 10.1021/acs.jchemed.6b00572
- [Assembling and Using a Simple, Low-Cost, Vacuum Filtration Apparatus That Operates without Electricity or Running Water](#) Fengxiu Zhang, Yiwei Hu, Yaling Jia, Yonghua Lu, and Guangxian Zhang, J. Chem. Educ., 2016, 93 (10), pp 1818–1820 DOI: 10.1021/acs.jchemed.5b00997
- [Rethinking Undergraduate Physical Chemistry Curricula](#), Stephen R. Miller, J. Chem. Educ., 2016, 93 (9), pp 1536–1542 DOI: 10.1021/acs.jchemed.5b00945
- [Teaching the Concept of Gibbs Energy Minimization through Its Application to Phase-Equilibrium Calculation](#), Romain Privat, Jean-Noël Jaubert, Etienne Berger, Lucie Coniglio, Cécile Lemaitre,

Dimitrios Meimaroglou, and Valérie Warth, *J. Chem. Educ.*, 2016, 93 (9), pp 1569–1577 DOI: 10.1021/acs.jchemed.6b00205

- [Interactively Applying the Variational Method to the Dihydrogen Molecule: Exploring Bonding and Antibonding](#), Vinícius Wilian D. Cruzeiro, Adrian Roitberg, and Nicolas C. Polfer, *J. Chem. Educ.*, 2016, 93 (9), pp 1578–1585 DOI: 10.1021/acs.jchemed.6b00017
- [Determination of Surface Tension of Surfactant Solutions through Capillary Rise Measurements: An Image-Processing Undergraduate Laboratory Experiment](#), Cristián Huck-Iriart, Ariel De-Candia, Javier Rodriguez, and Carlos Rinaldi, *J. Chem. Educ.*, 2016, 93 (9), pp 1647–1651 DOI: 10.1021/acs.jchemed.6b00128

## 2015

- [An Alternative Presentation of the Second Law of Thermodynamics](#) Sangyoub Lee, Kyusup Lee, and Jiyeon Lee, *J. Chem. Educ.*, 2015, 92 (4), pp 771–773 DOI: 10.1021/ed5007822
- [Measuring the Speed of Sound through Gases Using Nitrocellulose](#) Karen Sinclair Molek, Karl A. Reyes, Brandon A. Burnette, and Jacob R. Stepherson, *J. Chem. Educ.*, 2015, 92 (4), pp 762–766 DOI: 10.1021/ed400653t
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- [Hydrogen Storage Experiments for an Undergraduate Laboratory Course—Clean Energy: Hydrogen/Fuel Cells](#) Alla Bailey, Lisa Andrews, Ameya Khot, Lea Rubin, Jun Young, Thomas D. Allston, and Gerald A. Takacs, *J. Chem. Educ.*, 2015, 92 (4), pp 688–692 DOI: 10.1021/ed5006294
- [Are the Concepts of Dynamic Equilibrium and the Thermodynamic Criteria for Spontaneity, Nonspontaneity, and Equilibrium Compatible?](#) Lee J. Silverberg, Lionel M. Raff, *J. Chem. Educ.*, 2015, 92 (4), pp 655–659 DOI: 10.1021/ed500660j
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## 2014

- [Deconstructing Phase Diagram Calculations](#) Pierre Tomasini, *J. Chem. Educ.*, 2014, 91 (6), pp 934–936 DOI: 10.1021/ed400364s
- [Binary Solid–Liquid Phase Diagram of Phenol and t-Butanol: An Undergraduate Physical Chemistry Experiment](#) Xinhua Xu, Xiaogang Wang, and Meifen Wu, *J. Chem. Educ.*, 2014, 91 (6), pp 929–933 DOI: 10.1021/ed400598s
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- [Using a Spreadsheet To Solve the Schrödinger Equations for the Energies of the Ground](#)

- [Electronic State and the Two Lowest Excited States of H<sub>2</sub>](#) Yingbin Ge, Robert C. Rittenhouse, Jacob C. Buchanan, and Benjamin Livingston, *J. Chem. Educ.*, 2014, 91 (6), pp 853–859 DOI: 10.1021/ed400693p (? en Python ?)
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  - [Scent Transmutation: A New Way To Teach on Chemical Equilibrium, Distillation, and Dynamic Combinatorial Chemistry](#) Qing Ji, Nadia S. El-Hamdi, and Ognjen Š. Miljanić, *J. Chem. Educ.*, 2014, 91 (6), pp 830–833 DOI: 10.1021/ed400681w

## Dans Chemistry Education Research and Practice

- [University chemistry students' interpretations of multiple representations of the helium atom](#) Zahilyn D. Roche Allred and Stacey Lowery Bretz, *Chem. Educ. Res. Pract.*, 2019,20, 358-368 DOI: 10.1039/C8RP00296G
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  - cf. [What lies behind a graph?](#) By David Read, *Education in Chemistry*, 19/03/2020

## Springer

- [Some remarks concerning the thermodynamics of the simple ideal gas and related mathematical background](#), Láng, G.G. *ChemTexts* (2016) 2: 10. doi:10.1007/s40828-016-0028-2

## Divers

- [The hot chocolate effect might have practical application](#)
  - [Contactless, probeless and non-titrimetric determination of acid–base reactions using broadband acoustic resonance dissolution spectroscopy \(BARDS\)](#), M. Rizwan Ahmed, Sean McSweeney, Jacob Krüse, Bastiaan Vos and Dara Fitzpatrick, *Analyst*, 2018, 956-962. DOI : 10.1039/C7AN01447C
  - [A Century of ASME Steam Tables](#) Dec 14, 2021, Allan H. Harvey and James C. Bellows

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