

Edwar Davila Montenegro, Ph.D.

Materials Scientist | Physicist | Mathematician | STEM Educator

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Academic Profile

Materials scientist, physicist, and mathematician, currently pursuing an undergraduate degree in Computer Science. He works at the interface of polymeric nanocarriers, controlled drug delivery, computational chemistry, thermodynamics of computation, and science education. His research combines molecular modeling with experimental characterization to design and evaluate polymer-drug systems, while his work on neural computation investigates the physical and energetic limits of artificial intelligence. He also develops scientific software, leads interdisciplinary projects, mentors student teams in educational satellite and robotics programs, and communicates science to academic and public audiences.

Research interests: polymeric nanocarriers; controlled drug release; biomaterials; molecular docking; density functional theory; thermodynamics of computation; neural computation; energy efficiency in artificial intelligence; scientific software; nanomedicine; educational satellites; robotics; project-based STEM education.

Education

Ph.D. in Materials Science and Engineering

2020–2025

Federal University of Piauí (UFPI), Teresina, Brazil

Dissertation: *Advances in Polymeric Nanosystems for Controlled Drug Release: An Integrated Computational and Experimental Approach for the Delivery of the Anticancer Molecule QPhNO₂*. Advisor: Prof. Marcília Pinheiro da Costa; co-advisor: Prof. Heurison de Sousa e Silva. CAPES doctoral fellowship.

M.Sc. in Materials Science and Engineering

2018–2020

Federal University of Piauí (UFPI), Teresina, Brazil

Thesis: *Characterization of Drug-Carrier Nanoparticles for an Anticancer Agent through Second-Harmonic Scattering*. Advisor: Prof. Heurison de Sousa e Silva. CAPES master's fellowship.

Degree in Mathematics

Completed

Centro Universitário Leonardo da Vinci (UNIASSELVI), Brazil

Undergraduate degree in Mathematics, complementing an interdisciplinary background in the exact sciences and education.

Licentiate Degree in Physics

2011–2017

Federal Institute of Piauí (IFPI), Teresina, Brazil

Undergraduate monograph: *MAGLEV: A New Possibility for Space Exploration*. Advisor: Prof. Ayrton Vasconcelos Lima.

Undergraduate Degree in Computer Science

In progress

Centro Universitário Leonardo da Vinci (UNIASSELVI), Brazil

Current studies in computing, scientific programming, software development, and computational modeling.

Academic and Professional Appointments

Researcher

2018–present

Graduate Program in Materials Science and Engineering, UFPI

Research in polymeric nanosystems, nanomedicine, drug delivery, molecular modeling, and experimental materials characterization.

2015–present	Founder and Chief Executive Officer <i>Graviton Scientific Society</i> Leadership of research, scientific outreach, technological innovation, and student mentoring initiatives.
Current	Technology and Robotics Teacher <i>Great International School, Teresina</i> Project-based teaching in physics, mathematics, programming, robotics, embedded systems, and maker culture.
Current	Science and Technology Educator <i>Municipal Education Network of Teresina</i> Development and mentoring of applied STEM projects for basic education.
Current	Founder and Editor-in-Chief <i>Integra Scientia - Journal of Science Education and Project-Based Research</i> Editorial leadership for an open-access journal focused on science education and project-based research.

Peer-Reviewed Publications

- Montenegro, E. D.** (2026). “The Thermodynamic Cost of Neural Computation: From Landauer’s Bound to the Energetic Gap of Artificial Intelligence.” *Trends in Computer Science and Information Technology*, 11(3), 106–134. doi:10.17352/tcsit.000116.
- Nunes, J. M.; Costa, R. K. M.; **Montenegro, E. D.**; Pinheiro, D. P.; Rizzo, M. S.; Ferreira, P. M. P.; Oliveira, J. C.; da Silva Júnior, E. N.; Pessoa, C.; Lima, F. C. A.; Silva, H. S.; Costa, M. P. (2026). “In silico prediction, molecular docking, and in vitro inhibition of the topoisomerase I by a new naphthoquinone with anticancer potential.” *In Silico Research in Biomedicine*, 2, 100430. doi:10.1016/j.insr.2026.100430.
- Amos, Y.; **Montenegro, E. D.**; Rubaka, C.; Swai, H. (2026). “Fabrication and evaluation of quinine-loaded chitosan-polycaprolactone core-shell polymeric nanoparticles for the treatment of malaria: an in vitro and in silico study.” *Journal of Biomaterials Science, Polymer Edition*, 1–33. doi:10.1080/09205063.2026.2639582.
- Montenegro, E. D.**; Rizzo, M. S.; Silva, H. S.; Costa, M. P. (2025). “Development and Validation of NanoEDW 1.0: An Integrated Computational Tool for Drug Delivery Research and Nanotechnology Applications.” *J*, 8(4), 47. doi:10.3390/j8040047.
- Montenegro, E. D.**; Nunes, J. M.; Ramos, I. F. S.; Almeida, R. G.; da Silva Júnior, E. N.; Rizzo, M. S.; da Silva-Filho, E. C.; Ribeiro, A. B.; Silva, H. S.; Costa, M. P. (2025). “Characterization of the Interaction of a Novel Anticancer Molecule with PMMA, PCL, and PLGA Polymers via Computational Chemistry.” *Applied Sciences*, 15(1), 468. doi:10.3390/app15010468.
- Montenegro, E. D.**; Oliveira, S. C. S. D.; Souza Filho, C. A. G.; Pacheco, R. A.; Lima, B. V. C. (2025). “Innovación en Energía Solar: Prototipo de Generador Solar con Seguimiento Automatizado.” *Revista Innovación y Desarrollo Sostenible*, 5(2), 29–34. doi:10.47185/27113760.v5n2.159.
- Cláudio, C. F.; **Montenegro, E. D.**; Lima, Y. C. C. (2024). “Dispositivo de monitoramento da incidência de radiação UV solar: uma ferramenta de auxílio no combate ao câncer de pele.” *Revista FT*, 29(140), 30–31. doi:10.69849/revistaft/cl10202411302130.
- Borges de Souza, A.; **Montenegro, E. D.** (2022). “Aplicación de metodología MAKER y STEAM como catalizador para el desarrollo de proyectos de nano-satélites con aplicaciones a la exploración espacial en Brasil.” *Revista Innovación y Desarrollo Sostenible*, 3(1), 23–30. doi:10.47185/27113760.v3n1.82.

Research Software

2025	NanoEDW 1.0 <i>Open scientific software developed in Python</i> Integrated workflow for calibration curves, automated encapsulation-efficiency calculations, and fitting drug-release kinetics to Higuchi, Korsmeyer-Peppas, Weibull, and related models. Scientifically validated against spreadsheet and OriginPro workflows; see doi:10.3390/j8040047.
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Selected Conference Contributions

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- 2025 **A Computational Approach to Streamlining Drug Encapsulation Efficiency Analysis**
1st Seven Global Congress of Multidisciplinary Studies
 With H. S. Silva and M. P. Costa. [doi:10.56238/1stcongresssevenmultidisciplinarystudies-005](https://doi.org/10.56238/1stcongresssevenmultidisciplinarystudies-005).
- 2024 **Using Reverse Docking to Study Interactions between an Anticancer Molecule and Proteins in Cancer Cells**
VIII International One Health Congress and IV International Multiprofessional Health Symposium
 Conference-proceedings abstract, ISBN 978-65-272-1012-2.
- 2023 **Investigating Drug-Polymer Interactions of QPhNO₂, PCL, PLGA, and PMMA Using DFT Quantum-Chemical Calculations for Nanoencapsulation Applications**
Argentine Symposium on Polymers - SAP 2023
 International symposium contribution on computational screening of polymer-drug interactions.

Honors and Awards

- **2026 - Regional Champion, North/Northeast (Level 1):** IDBSaT project and the Niède Guidon mission; third consecutive regional title in educational satellite competition.
- **2024 - Regional Champion and National Runner-up (second place):** Brazilian Satellite Olympiad, student-team project mentorship.
- **2023 - Regional Champion and National Runner-up (second place):** Brazilian Satellite Olympiad, Greater and Cidade Olímpica teams.
- **2020 - First Place, National Stage:** Satellites + Artificial Intelligence Challenge, 17th National Science and Technology Week.

Books and Science Communication

Author and co-author of four books spanning scientific writing, space exploration, the public value of science, and the physical limits of artificial intelligence.

Montenegro, E. D. (2026). *Depois do Algoritmo: Informação, energia e os limites físicos do progresso*. Editora Bereshit, 169 pp.

Montenegro, E. D. (2023). *Os Cientistas Sempre Estarão na Linha de Frente*. 1st ed. Joinville, SC: Clube de Autores, 198 pp.

Montenegro, E. D. (2023). *Estradas Cósmicas*. 1st ed. Curitiba: Artêra Editorial, 145 pp.

Andrade, A. A. O.; **Montenegro, E. D.** (2020). *LaTeX para Cientistas*. 1st ed. Independently Published, 192 pp. ISBN 979-8567015551.

Methods and Technical Expertise

Computational research	Python; molecular docking; reverse docking; density functional theory; molecular-property analysis; data visualization; kinetic-model fitting.
Experimental research	Polymeric nanoparticles; drug encapsulation; controlled-release systems; second-harmonic scattering; materials characterization.
Education and prototyping	Robotics; Arduino; embedded systems; telemetry; educational satellites; Maker and STEAM methodologies; project-based learning.
Scientific communication	Academic writing; LaTeX; editorial work; interdisciplinary project mentoring; public science communication.

The publication list and academic links in this CV were reviewed against the author's public academic records and official website in October 2026.