



Igor Daniel de Araujo Evangelista

Postdoctoral Scholar, Photon Science, SLAC

Bio

BIO

Dr. Evangelista's primary research focus lies in computational modeling and theoretical analysis of semiconductor materials using advanced quantum mechanical methods, including Density Functional Theory, Quantum Monte Carlo, and ab-initio Molecular Dynamics. Evangelista investigates the electronic, structural, and mechanical properties of materials, collaborating closely with experimental groups to bridge theoretical predictions with empirical results. He is also interested in the development of empirical potentials and enhancing materials modeling through the application of machine learning techniques.

Evangelista entered the Department of Materials Science and Engineering at the University of Delaware as a Ph.D. candidate in 2018, after completing an master degree in Physics 2016-2018 at Federal Fluminense University (Brazil). Recent work includes collaborations with experimental groups to bridge theoretical predictions with empirical results, as well as applying machine learning to creating of empirical potentials to accelerate materials modeling. Evangelista has also contributed to understanding electron mobility in metal-oxide semiconductors and strain effects in two-dimensional materials. These studies showcase his expertise in electronic structure and materials design for next-generation semiconductor technologies.

STANFORD ADVISORS

- Piero Pianetta, Postdoctoral Faculty Sponsor
- Kirsten Winther, Postdoctoral Research Mentor

LINKS

- <https://scholar.google.com/citations?user=8UWI2sMAAAAJ&hl=en&oi=sra>: <https://scholar.google.com/citations?user=8UWI2sMAAAAJ&hl=en&oi=sra>

Publications

PUBLICATIONS

- **Phase stability and transition behaviors of (Bi_xIn_{1-x})₂Se₃ alloy** *APPLIED PHYSICS LETTERS*
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- **Defect Stability in CdTe Based on Formation Energies and Migration Barriers** *JOURNAL OF PHYSICAL CHEMISTRY C*
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- **Doping and defects in wide-band-gap perovskite semiconductors**
Janotti, A., Chatratin, I., Evangelista, I.

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SPIE-INT SOC OPTICAL ENGINEERING.2025

- **Large Rashba spin splittings in bulk and monolayer of BiAs** *PHYSICAL REVIEW MATERIALS*
Zubair, M., Evangelista, I., Khalid, S., Medasani, B., Janotti, A.
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- **Self-compensation of group-V acceptors in CdTe**
Janotti, A., Chatratin, I., Evangelista, I., IEEE
IEEE.2024: 1149
- **Doping the Undopable: Hybrid Molecular Beam Epitaxy Growth, n-Type Doping, and Field-Effect Transistor Using CaSnO₃**
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2023; 17 (17): 16912-16922
- **Structural Phase Transitions between Layered Indium Selenide for Integrated Photonic Memory** *ADVANCED MATERIALS*
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