

# JAN ESTRADA PABON

370 Lancaster Ave. Haverford PA 19071

939-253-7902 | jdep@stanford.edu

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## Education

**Stanford University:** Stanford, CA

PhD in Chemistry, concentration in theoretical chemistry

EDGE Fellow

*Graduation date: TBD*

**Haverford College:** Haverford, PA

Bachelor's in chemistry, concentration in Scientific Computing

Padín Scholar, Questbridge scholar

Relevant coursework: Physical Chemistry, Modelling thermodynamics through python

Organic Chemistry, Multivariable Calculus, Physical Chemistry,

Quantum Chemistry, Linear Algebra

GPA: 3.60

*Graduation date: May 2021*

**Saint John's School:** San Juan, PR

National Honor Society member, National Hispanic recognition

Program, French Honor Society, AP Scholar

*Graduation date: May 2017*

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## Experience

**Stanford University** | *Graduate Teaching Assistant*

*September 2021 – May 2022*

- **Mentored** a core of 50+ students for 3 college quarters
- Assisted in the **development of course material** such as exam questions and laboratory procedures

**IBM** | *Research Intern*

*June 2020 – August 2020*

As part of a team working on improving computational drug discovery...

- Built 700+ **interpretable QSAR deep learning models**
- **Optimized** deep learning models through **stochastic processes**
- Developed **protein-ligand system visualizations** from protein contact maps
- **Automated** and **parallelized** training of **deep learning models** on protein-ligand complexes

**Haverford College** | *Computational researcher*

*May 2018 – Present*

As part of a program that aimed to **improve** current **protein stability predictors** through computation...

- Analyzed a dataset of more than 100,000 proteins through **Python**
- Used sci-kit learn's **machine learning** algorithms such as **Random Forest Classifier, Scalar Vector Machine**
- Wrangled with a covariant **high dimensional** dataset
- **Created 17 protein descriptors** approximating configurational entropy
- Ran **Linear** and **Logistic regression** models on data
- Worked with a community of sixty-three investigators while handling an individual project.

As part of a program that aimed to **create new solar panel materials** through machine learning assisted discovery...

- Applied **machine learning auditing** techniques to **extract** meaningful **chemical insight** from model predictions

- Implemented a unique **model-on-model auditing method** where an interpretable model is trained on a complex model in order to approximate performance

**Haverford College** | *Member of Faculty Search Committee*

*August 2019 – December 2019*

- Served as a liaison between student body and incoming prospective faculty
- Gathered student body opinion on candidates and provided a compiled synopsis for the Hiring Committee to evaluate.

**MAST** | *Science tutor*

*February 2018 – May 2018*

- Taught high school students about topics including engineering, chemistry, programming, anatomy, and psychology
- Collaborated with a group of ten tutors and supervisors in order to maintain an engaging learning environment

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### Skills

- Mastery of **Python, Jupyter, Unix Shell, Matplotlib, Scikit-learn, Pandas, MDTraj, Psi4, ChemDraw, PyMol, Origin, LoggerPro, C-Sharp, TensorFlow, PyTorch, Bash, ProDy, Openbabel, Networkx**
- Knowledgeable on **machine learning** (SVM, RandomForestClassifier, K-NN), **regression** (Linear, Logistic, Lasso), and **feature selection** (K-Best, Variance Threshold)

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### Projects

- **Test-Harness** (Contributor): Implemented SHAP and BBA as methods for auditing black box models. Implemented a unique Model-on-model interpreter, where an interpretable model is fit on a complex one in order to approximate its performance. (<https://gitlab.sd2e.org/sd2program/test-harness>)
- **IPython-Mathematica** (Owner): Implemented an integration of Mathematica into Python and applied it to Multivariable Calculus problems in order to test its advantages ([https://github.com/jandestrada/IPython\\_Mathematica](https://github.com/jandestrada/IPython_Mathematica))

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### Publications

- (1) [Jan D. Estrada Pabon](#); Hugh Haddox; Greg van Aken; Ian M. Pendleton; Hamed Eramian; Jed Singer; Joshua Schrier\*. The role of configurational entropy in miniprotein stability. J. Phys. Chem. **2020**
- (2) Jeffrey K. Weber, Joseph A. Morrone, Sugato Bagchi, [Jan D. Estrada Pabon](#), Seung-gu Kang, Leili Zhang, and Wendy D. Cornell. Simplified, Interpretable Graph Convolutional Neural Networks for Small Molecule Activity Prediction. J Computer-Aided Molecular Design. **2021**