Omar A. Ashour

Postdoctoral Researcher, LBNL

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Education

2019 – 2025 **PhD, Physics**, University of California, Berkeley.
Dissertation Dark Matter Couture: Designer Targets and Tailored Detectors for Next-Generation Searches
Advisor Sinéad M. Griffin

2019 – 2020 **MA, Physics**, University of California, Berkeley.

2017 – 2019 **MS, Applied Physics**, University of California, Berkeley.
Thesis The Nonlinear Schrödinger Hierarchy: from Quasi Rogue Waves to Nonlinear Talbot Carpets

2013 – 2017 **BS, Electrical Engineering (Optics)**, Texas A&M University, *Summa Cum Laude*.
Thesis Maximal Intensity Higher-Order Breathers of the Nonlinear Schrödinger Equation

Professional Experience

07/2025 – **Postdoctoral Researcher**, *Computing Sciences Area and Molecular Foundry*.
Lawrence Berkeley National Laboratory, Berkeley, CA

Interests
- Catastrophe theory and statistical mechanics of feature superposition and polysemanticity.
- Information-geometric, physically inspired generalization of flow models.
- Generative deep models for amorphous materials and RNA/protein folding.
- Persistent (co)-homology for disordered systems.

Publications and Preprints

⋆ Equal Contribution † Corresponding Author

2025 Guy C. Moore, Matthew K. Horton, Aaron D. Kaplan, **Omar A. Ashour**, Sinéad M. Griffin, and Kristin A. Persson. Noncollinear ground states of solids with a source-free exchange correlation functional, *Phys. Rev. B*, **111**, 094417 (2025).

2025 Thomas F. Harrelson, Ibrahim Hajar, **Omar A. Ashour**, and Sinéad M. Griffin. Theoretical investigation of decoherence channels in athermal phonon sensors, *J. Phys. Condens. Matter*, **37**, 015002 (2025).

2024 Nicholas Dale⋆, **Omar A. Ashour**⋆, Marc Vila, Justin Fox, Resham Regmi, Alexei Fedorov, Alexander Stibor, Nirmal Ghimire, and Sinéad M. Griffin. Non-relativistic spin splitting above and below the fermi level in a *g*-wave altermagnet (2024). [arXiv:2411.18761]

2024 **Omar A. Ashour**† and Sinéad M. Griffin. Pressure-tunable targets for light dark matter direct detection: the case of solid helium (2024). [arXiv:2409.02439]

2024 Na Hyun Jo*, **Omar A. Ashour***, Zhixue Shu, Chris Jozwiak, Aaron Bostwick, Sae Hee Ryu, Kai Sun, Tai Kong, Sinéad M. Griffin, and Eli Rotenberg. Effects of strain, defects, and interactions on the topological properties of $HfTe_5$, *Phys. Rev. B*, **109**, 235122 (2024), ***Editor's Suggestion***.

2022 Stanko N. Nikolić, Sarah Alwashahi, **Omar A. Ashour**, Siu A. Chin, Najdan B. Aleksić, and Milivoj R. Belić. Multi-elliptic rogue wave clusters of the nonlinear Schrödinger equation on different backgrounds, *Nonlinear Dynamics*, **108**, 479–490 (2022).

2022 **Omar A. Ashour**†, Siu A. Chin, Stanko N. Nikolić, and Milivoj R. Belić. Higher-order breathers as quasi-rogue waves on a periodic background, *Nonlinear Dynamics*, **107**, 3819–3832 (2022).

2022 Thais Chagas*, **Omar A. Ashour***, Guilherme Ribeiro, Wendell Silva, Zhenglu Li, Rogério Magalhães-Paniago, Yves Petroff, and Steven G. Louie. Multiple strong topological gaps and hexagonal warping in Bi_4Te_3, *Physical Review B*, **105**, L081409 (2022).

2022 Milivoj R. Belić, Stanko N. Nikolić, **Omar A. Ashour**, and Najdan B. Aleksić. On different aspects of the optical rogue waves nature, *Nonlinear Dynamics*, **108**, 1655–1670 (2022).

2021 **Omar A. Ashour**†. NonlinearSchrodinger: higher-order algorithms and Darboux transformations for nonlinear Schrödinger equations (2021). [arXiv:2103.14469]

2019 Stanko N. Nikolić, **Omar A. Ashour**, Najdan B. Aleksić, Yiqi Zhang, Milivoj R. Belić, and Siu A. Chin. Talbot carpets by rogue waves of extended nonlinear Schrödinger equations, *Nonlinear Dynamics*, **97**, 1215–1225 (2019).

2019 Stanko N. Nikolić, **Omar A. Ashour**, Najdan B. Aleksić, Milivoj R. Belić, and Siu A. Chin. Breathers, solitons and rogue waves of the quintic nonlinear Schrödinger equation on various backgrounds, *Nonlinear Dynamics*, **95**, 2855–2865 (2019).

2017 Stanko N. Nikolić, Najdan B. Aleksić, **Omar A. Ashour**, Milivoj R. Belić, and Siu A. Chin. Systematic generation of higher-order solitons and breathers of the Hirota equation on different backgrounds, *Nonlinear Dynamics*, **89**, 1637–1649 (2017).

2017 Runze Li, **Omar A. Ashour**, Jie Chen, H. E. Elsayed-Ali, and Peter M. Rentzepis. Femtosecond laser induced structural dynamics and melting of Cu (111) single crystal: an ultrafast time-resolved x-ray diffraction study, *Journal of Applied Physics*, **121**, 055102 (2017).

2017 Siu A. Chin, **Omar A. Ashour**, Stanko N. Nikolić, and Milivoj R. Belić. Peak-height formula for higher-order breathers of the nonlinear Schrödinger equation on non-uniform backgrounds, *Physical Review E*, **95**, 012211 (2017).

2016 Siu A. Chin, **Omar A. Ashour**, Stanko N. Nikolić, and Milivoj R. Belić. Maximal intensity higher-order Akhmediev breathers of the nonlinear Schrödinger equation and their systematic generation, *Physics Letters A*, **380**, 3625–3629 (2016).

2015 Siu A. Chin, **Omar A. Ashour**, and Milivoj R. Belić. Anatomy of the Akhmediev breather: cascading instability, first formation time, and Fermi-Pasta-Ulam recurrence, *Physical Review E*, **92**, 063202 (2015).

Manuscripts in Preparation

- **Omar A. Ashour** and Sinéad M. Griffin. Topological transition sensors in antiferromagnetic and topological crystalline insulators.

- J. Wayne Mullinax, **Omar A. Ashour**, Antonios Alvertis, Daniel Gibney, Katherine Klymko, and Norman Tubman. Exploring the variational quantum eigensolver with one-body reduced density matrices.
- Jan Balewski, Alexey Khudorozhkov, **Omar A. Ashour**, Siva Darbha, Pedro LS Lopes, Sheng-Tao Wang, Daan Camps, Katherine Klymko, Milan Kornjača, and Fangli Liu. Observation of an anomaly in the statistics of Kibble-Zurek defects.
- **Omar A. Ashour** and Sinéad M. Griffin. Topological transition sensors for phonon- and magnon-mediated particle detection and quantum sensing.

Research Experience

2024	**Quantum @ NERSC, Lawrence Berkeley National Lab**, Berkeley, CA.
PIs	Katherine Klymko (LBL) and Norman Tubman (NASA QuAIL)
Topics	Development of VQE variants with DFT- and RDMFT-based cost functions (with NASA).
	Quantum simulation of the Kibble-Zurek mechanism in 1D neutral atom chains (with QuEra).
2021 – 2025	**Molecular Foundry and Materials Sciences Division, Berkeley Lab**, Berkeley, CA.
PI	Sinéad M. Griffin
Topic	Leveraging quantum materials for novel quantum sensing schemes and dark matter detection.
2019 – 2021	**Physics Department, UC Berkeley**, Berkeley, CA.
PI	Steven G. Louie
Topic	DFT and GW calculations of low-dimensional materials (e.g., TMDs).
2017 – 2018	**NSF Nanoscale Science & Engineering Center, UC Berkeley**, Berkeley, CA.
PI	Xiang Zhang
Topic	Ultrafast spectroscopy of low-dimensional materials.
2014 – 2017	**Department of Physics and Astronomy, Texas A&M University**, College Station, TX.
PIs	Siu A. Chin and Milivoj R. Belić
Topic	Mathematical and computational nonlinear physics.
2016 – 2017	**Texas A&M Engineering Experiment Station (TEES)**, College Station, TX.
PI	Peter M. Rentzepis
Topic	Ultrafast X-ray studies of thin films, and ultrafast optical studies of biological molecules.
2015	**Institute of Electronic Structure and Laser (IESL-FORTH)**, Heraklion, Greece.
PI	Stelios Tzortzakis
Topic	Femotosecond laser machining of low-loss waveguides.

Fellowships and Competitive Awards

2025	Finalist for the **University of California President's Postdoctoral Fellowship**.
2025	Elected to full membership of **Sigma Xi**.
2024	**Ovshinsky Travel Award**, Division of Materials Physics, American Physical Society.
2018 – 2019	**Anselmo J. Macchi Graduate Fellowship**, UC Berkeley.
2017 – 2019	**Berkeley Graduate Fellowship**, UC Berkeley.
2017 – 2018	**Cornell Graduate Fellowship** (declined), Cornell University.

2016 **Richard E. Ewing Award** for excellence in undergraduate research, Texas A&M University.

2014, '15, '17 **Gathright Scholar Award** for outstanding academic achievement, Texas A&M University.

2016 **Takreem Award** for undergraduate research, Qatar Foundation for Education and Science.

2014 – 2017 **Merit Scholarship**, Qatar Foundation for Education and Science.

Selected Software Packages (Lead or Sole Developer)

GitHub **DarkMAGIC** [Python/MPI/Numba].
Parallel, high-throughput package for calculating phonon and magnon interactions with general dark matter models using first-principles calculations, model Hamiltonians, and effective field theory.

GitHub `pymatgen.io.espresso` [Python].
Exploiting ducktyping, this package elevates Quantum ESPRESSO (QE) to a first-class citizen in the `pymatgen` ecosystem, enabling VASP-based packages to fully support QE with just two lines of code.

GitHub **Quesadilla** [Python/Fortran].
Symmetry-based implementation of linear-scaling nondiagonal supercells for phonons, with a `phonopy` interface.

GitHub `NonlinearSchrodinger.jl` [Julia].
arXiv Highly-performant package for solving nonlinear Schroödinger-type partial differential equations using numerical and analytical algorithms.

Contributions I have contributed to a variety of scientific packages in C/C++, FORTRAN, CUDA, MPI, OpenMP, and OpenACC. Examples include `pymatgen`, `sumo`, and VASP patches.

Service and Outreach (Since 2021)

Aug. 2024 **Symposium Organization:** I proposed and organized a symposium, *Next-Generation Quantum Materials for Quantum Computing and Sensing* at the annual Molecular Foundry User Meeting, featuring invited and contributed talks from across the U.S.

'21, '22, '23, '24 **Griffin Group MVP**: voted by peers in my research group as the year's "most valuable physicist" for fostering a collaborative and inclusive environment.

2021 – **Educational Resources**: I maintain a popular website, https://ashour.dev, which features my comprehensive notes on group theory, condensed matter physics, density functional theory, and other academic topics. The site also includes tutorials and practical guides on several aspects of computational solid-state physics, attracting over 80,000 monthly visits.

2021 – **Undergraduate Mentoring**: I am involved in mentoring several undergraduate students, and have trained and lectured to summer intern cohorts at Berkeley Lab.