

[PHYSICAL REVIEW MATERIALS \(/PRMATERIALS/\)](#)

- [Highlights \(/prmaterials/highlights\)](#)
 [Recent \(/prmaterials/recent\)](#)
 [Accepted \(/prmaterials/accepted\)](#)
[Research Updates \(/prmaterials/research_updates\)](#)
 [Collections \(/prmaterials/collections\)](#)
 [Authors \(/prmaterials/authors\)](#)
[Referees \(/prmaterials/referees\)](#)
 [Search \(/search\)](#)
 [About \(/prmaterials/about\)](#)
 [Editorial Team \(/prmaterials/staff\)](#)
 [🔔 \(/feeds\)](#)

Excitonic effects in graphene-like C_3N

Miki Bonacci, Matteo Zanfagnini, Elisa Molinari, Alice Ruini, Marilia J. Caldas, Andrea Ferretti, and Daniele Varsano
 Phys. Rev. Materials **6**, 034009 – Published 23 March 2022



(https://www.altmetric.com/details.php?domain=journals.aps.org&citation_id=125320203)

More

Article

- [PDF \(/prmaterials/pdf/10.1103/PhysRevMaterials.6.034009\)](#)
 [HTML \(/prmaterials/abstract/10.1103/PhysRevMaterials.6.034009#fulltext\)](#)
[Export Citation \(/prmaterials/export/10.1103/PhysRevMaterials.6.034009\)](#)



ABSTRACT

AUTHORS

ARTICLE TEXT

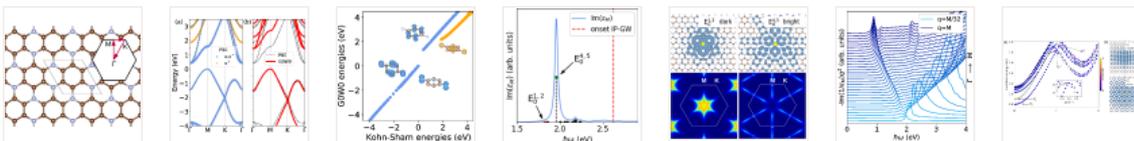
- [INTRODUCTION](#)
[METHODS](#)
[RESULTS AND DISCUSSION](#)
[CONCLUSIONS](#)
[ACKNOWLEDGMENTS](#)

SUPPLEMENTAL MATERIAL

REFERENCES

ABSTRACT

Monolayer C_3N is an emerging two-dimensional indirect band gap semiconductor with interesting mechanical, thermal, and electronic properties. In this paper we present a description of C_3N electronic and dielectric properties, focusing on the so-called momentum-resolved exciton band structure. Excitation energies and oscillator strengths are computed in order to characterize bright and dark states, and discussed also with respect to the crystal symmetry. Activation of excitonic states is observed for finite transferred momenta: Indeed, we find an active indirect exciton at ~ 0.9 eV, significantly lower than the direct optical gap of 1.96 eV, with excitonic binding energies in the range 0.6–0.9 eV for the lowest states. As for other 2D materials, we find a quasilinear excitonic dispersion close to Γ , which however shows a downward convexity related to the indirect band gap of C_3N as well as to the dark nature of the involved excitons.



Received 16 November 2021 Accepted 8 March 2022

DOI: <https://doi.org/10.1103/PhysRevMaterials.6.034009>

©2022 American Physical Society

Physics Subject Headings (PhySH)

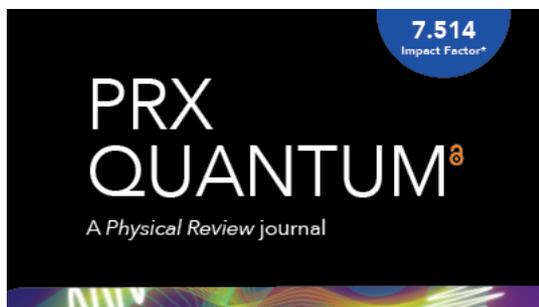
Research Areas



[Log in with individual APS Journal Account » \(https://journals.aps.org/login\)](https://journals.aps.org/login)

[Log in with a username/password provided by your institution » \(/login_inst_user?rt=https%3A%2F%2Fjournals.aps.org%2Fprmaterials%2Fabstract%2F10.1103%2FPhysRevMaterials.6.034009\)](https://journals.aps.org/login_inst_user?rt=https%3A%2F%2Fjournals.aps.org%2Fprmaterials%2Fabstract%2F10.1103%2FPhysRevMaterials.6.034009)

[Get access through a U.S. public or high school library » \(/free-access-for-us-public-and-high-school-libraries\)](#)



Sign up to receive regular email alerts from *Physical Review Materials*

Sign up [\(\(https://info.aps.org/journals-emails\)\)](https://info.aps.org/journals-emails)

[APS \(https://www.aps.org/\)](https://www.aps.org/) | [Current Issue \(\(prmaterials/issues/current\)\)](https://prmaterials/issues/current) | [Earlier Issues \(\(prmaterials/issues\)\)](https://prmaterials/issues) | [News & Announcements \(\(prmaterials/edannounce\)\)](https://prmaterials/edannounce) | [About this Journal \(\(prmaterials/about\)\)](https://prmaterials/about) | [Journal Staff \(\(prmaterials/staff\)\)](https://prmaterials/staff) | [About the Journals \(\(about\)\) \(https://www.facebook.com/apsphysics\)](https://www.facebook.com/apsphysics) | [\(\(https://twitter.com/APSphysics\)\)](https://twitter.com/APSphysics) | [Join APS \(https://www.aps.org/membership/join.cfm\)](https://www.aps.org/membership/join.cfm)

AUTHORS

[General Information \(\(prmaterials/authors\)\)](https://prmaterials/authors)
[Submit a Manuscript \(https://authors.aps.org/Submissions/\)](https://authors.aps.org/Submissions/)
[Publication Rights \(\(pub_rights.html\)\)](https://pub.rights.html)

REFEREES

[General Information \(\(prmaterials/referees\)\)](https://prmaterials/referees)
[Submit a Report \(http://referees.aps.org/\)](http://referees.aps.org/)
[Update Your Information \(http://referees.aps.org/\)](http://referees.aps.org/)

[Open Access \(/open_access.html\)](#)

[Policies & Practices \(/pmaterials/authors/editorial-policies-practices\)](#)

[Policies & Practices \(/pmaterials/authors/editorial-policies-practices\)](#)

[Referee FAQ \(/referees/faq.html\)](#)

[Tips for Authors \(/authors/tips-authors-physical-review-physical-review-letters\)](#)

[Guidelines for Referees \(/pmaterials/referees/advice-referees-physical-review-materials\)](#)

[Professional Conduct \(/authors/professional-conduct-ethics\)](#)

[Outstanding Referees \(/OutstandingReferees\)](#)

LIBRARIANS

[General Information \(https://librarians.aps.org/\)](https://librarians.aps.org/)

[Subscriptions \(https://librarians.aps.org/subscriptions\)](https://librarians.aps.org/subscriptions)

[Online License Agreement \(https://librarians.aps.org/sitelicense.pdf\)](https://librarians.aps.org/sitelicense.pdf)

[Usage Statistics \(http://counter.aps.org/\)](http://counter.aps.org/)

[Your Account \(https://librarians.aps.org/account\)](https://librarians.aps.org/account)

STUDENTS

[Physics \(https://physics.aps.org\)](https://physics.aps.org)

[PhysicsCentral \(http://www.physicscentral.com/\)](http://www.physicscentral.com/)

[Student Membership \(https://www.aps.org/membership/student.cfm\)](https://www.aps.org/membership/student.cfm)

APS MEMBERS

[Subscriptions \(https://www.aps.org/membership/aps-publications.cfm\)](https://www.aps.org/membership/aps-publications.cfm)

[Article Packs \(https://journals.aps.org/article-packs\)](https://journals.aps.org/article-packs)

[Membership \(https://www.aps.org/membership/index.cfm\)](https://www.aps.org/membership/index.cfm)

[FAQ \(https://www.aps.org/membership/faq.cfm\)](https://www.aps.org/membership/faq.cfm)

[APS News \(https://www.aps.org/publications/apsnews/index.cfm\)](https://www.aps.org/publications/apsnews/index.cfm)

[Meetings & Events \(https://www.aps.org/meetings/index.cfm\)](https://www.aps.org/meetings/index.cfm)

[Privacy \(https://www.aps.org/about/webpolicies.cfm#privacy\)](https://www.aps.org/about/webpolicies.cfm#privacy)

[Policies \(/policies\)](#)

[Contact Information \(/contact.html\)](#)

[Feedback \(mailto:feedback@aps.org\)](mailto:feedback@aps.org)

ISSN 2475-9953 (online). ©2022 American Physical Society (<https://www.aps.org/>). All rights reserved. *Physical Review Materials*™ is a trademark of the American Physical Society, registered in the United States, Canada, European Union, and Japan. The *APS Physics logo* and *Physics logo* are trademarks of the American Physical Society. Information about registration may be found [here \(/legal\)](#). Use of the American Physical Society websites and journals implies that the user has read and agrees to our [Terms and Conditions \(/info/terms.html\)](#) and any applicable [Subscription Agreement \(https://librarians.aps.org/sitelicense.pdf\)](#).