



Mass Spectrometers for
Catalysis Research

Click Here

AIP

The Journal of Chemical Physics

[HOME](#)[BROWSE](#)[MORE ▼](#)

[Home](#) > [The Journal of Chemical Physics](#) > [Volume 134, Issue 17](#) > [10.1063/1.3584680](#)

[< PREV](#)[NEXT >](#)

Published Online: 05 May 2011

Accepted: April 2011

Anhydrous crystals of DNA bases are wide gap semiconductors

J. Chem. Phys. **134**, 175101 (2011); <https://doi.org/10.1063/1.3584680>

F. F. Maia Jr.^{1,2}, V. N. Freire², E. W. S. Caetano^{3, a)}, D. L. Azevedo^{4,5}, F. A. M. Sales^{2,4}, and E. L. Albuquerque⁴

[View Affiliations](#)



Topics ▼



PDF

ABSTRACT

We present the structural, electronic, and optical properties of anhydrous crystals of DNA nucleobases (guanine, adenine, cytosine, and thymine) found after DFT (Density Functional Theory) calculations within the local density approximation, as well as experimental measurements of optical absorption for powders of these crystals. Guanine and cytosine (adenine and thymine) anhydrous crystals are predicted from the DFT simulations to be direct (indirect) band gap semiconductors, with values 2.68 eV and 3.30 eV (2.83 eV and 3.22 eV), respectively, while the experimentally estimated band gaps we have measured are 3.83 eV and 3.84 eV (3.89 eV and 4.07 eV), in the same order. The electronic effective masses we have obtained at band extremes show that, at low temperatures, these crystals behave like wide gap semiconductors for electrons moving along the nucleobases stacking direction, while the hole transport are somewhat limited. Lastly, the calculated electronic dielectric functions of DNA nucleobases crystals in the parallel and perpendicular directions to the stacking planes exhibit a high degree of anisotropy (except cytosine), in agreement with published experimental results.

- Original article: [JCP: BioChemical Physics 5 \(5\), 05B601 \(2011\)](#)

ACKNOWLEDGMENTS

E.L.A. and V.N.F. are senior researchers from the Brazilian National Research Council (CNPq), and would like to acknowledge the financial support received during the development of this work from the Brazilian



Nano(Bio)Simes project 573925/2008-9, and FAPERN-CNPq (Pronex).

E.W.S.C. received financial support from CNPq projects 304338/2007-9 and 482051/2007-8.

SELECT YOUR ACCESS

INDIVIDUAL ACCESS

If you have an individual subscription, a subscription provided by one of AIP's Member Societies, have claimed access to a Conference Proceeding, or have made an individual purchase, sign in below.

Username:

Password

☐ Remember me

LOG IN

[Forgot password?](#)

INSTITUTIONAL ACCESS

[Log in via Open Athens](#)

[Log in via Shibboleth](#)

PURCHASE

☐ Standard PPV for \$30.00

ADD TO CART



PDF



Where in the **world** is AIP Publishing?



Resources

[AUTHOR](#)

[LIBRARIAN](#)

[ADVERTISER](#)

General Information

[ABOUT](#)

[CONTACT](#)

[HELP](#)

[PRIVACY POLICY](#)

[TERMS OF USE](#)

FOLLOW AIP PUBLISHING:



 [PDF](#)

Website © 2019 AIP Publishing LLC.

Article copyright remains as
specified within the article.

Scitation



PDF