AUTHOR COMMENTARIES - From Special Topics

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Oded Hod, Gustavo Scuseria, & Veronica Barone

From the Special Topic of Graphene

*According to our Special Topics analysis on Graphene, a key paper in the Research Front Map on Graphene Nanoribbons is "Electronic structure and stability of semiconducting graphene nanoribbons," (*Nano Lett*. 6[12]: 2748-54, 13 December 2006). In* Essential Science Indicators℠ *from Thomson Reuters, this paper garnered 70 citations up to October 31, 2008. In the* Web of Science®, *this paper currently has 80 citations.*

The paper's authors are Prof. Gustavo Scuseria, who is the Robert A. Welch Professor of Chemistry at Rice University; Dr. Veronica Barone, who is an Adjunct Assistant Professor in the Department of Physics at Central Michigan University; and Dr. Oded Hod, who is a Senior Lecturer in the School of Chemistry at Tel-Aviv University.

In the interview below,* ScienceWatch.com *talks with Dr. Hod about the work he and his colleagues did on this paper.

SW: Would you please describe the significance of your paper and why it is highly cited?

Our paper presents the first calculation, based on screened-hybrid density functional theory, of the electronic and structural properties of semi-conducting graphene nanoribbons. Our findings reveal important differences between previous calculations, based on lower-level theories, and our more accurate results obtained using first-principles methods. We stress the importance of controlling the width of narrow graphene nanoribbons aiming to tailor their electronic properties, and we demonstrate, for the first time, that the nature of the edges can be elucidated by studying their optical signature.

Our predictions were verified experimentally by several research groups, indicating the impressive accuracy of the state-of-the-art screened-hybrid density functional known as HSE, which was developed in the Scuseria group.

SW: How did you become involved in this research, and were there any particular successes or obstacles that stand out?

I was involved in the research by my post-doc host, Prof. Gustavo E. Scuseria, who has considerable experience in both developing electronic structure methods and applying them to a variety of systems including carbon-based materials. Prof. Scuseria understood the

importance of the field while reading recent literature and noticed the potential of using the methods developed in our group for studying the physical properties of graphene nanoribbons. My fruitful collaboration with Dr. Veronica Barone led to the success of this project and, as stated above, one of the main achievements was that our theoretical predictions were verified experimentally shortly after their publication.

SW: Where do you see your research and the broader field leading in the future?

Recently, I moved from Rice University in Houston, Texas, where I concluded my post-doc term, to Tel-Aviv University in Israel, where I have accepted a position as a faculty member at the School of Chemistry. In the field of graphene nanoribbons I continue my research on the electronic, magnetic, and electro-mechanical properties of these fascinating systems.

Furthermore, I study the chemical adsorption of contaminants on graphene nanoribbons in order to estimate the feasibility of their use as ultra-sensitive and highly reliable chemical sensors. I believe that in the near future we will find a growing number of proof-of-concept studies showing the ability to use this versatile material in electronic, spintronic, and nano-mechanical devices.

SW: What are the implications of your work for this field?

Since the tools that we have are extremely suitable for the treatment of graphene-based materials, our prediction power enables us to design, support, and direct experimental efforts in the field. I am currently in the process of forming several cooperations with experimental groups in this field, aiming at combining our computational power with their experimental expertise.

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Oded Hod, Gustavo Scuseria, & Veronica Barone's current most-cited paper in *Essential Science Indicators*, with 64 cites:

Barone V, Hod O, Scuseria GE, "Electronic structure and stability of semiconducting graphene nanoribbons," *Nano Lett.* 6(12): 2748-54, 13 December 2006. Source: *Essential Science Indicators* from Thomson Reuters.

Additional Information:

Gustavo Scuseria is featured in *ISIHighlyCited.com*.

Keywords: semiconducting graphene nanoribbons, structure, stability, screened-hybrid density functional theory, electronic properties, optical signature, chemical adsorption.

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