SYLVIO CANUTO

Festschrift

A scientist and a friend

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LF
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CONSELHO EDITORIAL

CURRÍCULO ACADÊMICO DO PROF. SYLVIO CANUTO

Formação Acadêmica

- Bacharel e Mestre em Física pela Universidade de Brasília (UnB).
- Doutorado em Física pela Universidade de Uppsala, Suécia (1979).

Carreira Acadêmica

- Professor do Departamento de Física da UFPE (1980–1994).
    - Professor Titular (1989).
    - Chefe de Departamento (1989–1991).
- Professor Titular do Instituto de Física da USP (1994–2025).
    - Chefe do Departamento de Física dos Materiais (2004–2006).
    - Chefe do Departamento de Física Geral (2008–2012).
    - Professor Sênior (2025).
    - Pesquisador 1A do CNPq continuamente desde 2000.

Reconhecimentos e Honrarias

- Ordem Nacional do Mérito Científico, classe de Comendador (2018).
- Membro Titular da Academia Brasileira de Ciências (ABC), da Academia de Ciências do Estado de São Paulo (ACIESP) e da TWAS (The World Academy of Sciences).

Atuação Institucional

- Pró-Reitor de Pesquisa da USP (2018–2022).
- Presidente da Sociedade Brasileira de Física.
- Coordenador Geral de Ciências, Humanidades e Artes na FAPESP.
- Membro e Presidente do Comitê Assessor de Física e Astronomia do CNPq (2000–2002).
- Coordenador da Área de Astronomia e Física na CAPES (2011–2018).
- Representante do CTC-ES no Conselho Superior da CAPES (2015–2018).

Atuação Editorial

- Co-Editor-in-Chief do periódico *Spectrochimica Acta A: Molecular and Biomolecular Spectroscopy* (Elsevier) desde 2016.

Produção Científica

- Cerca de 300 artigos publicados em periódicos internacionais.
- Índice H = 47, com mais de 8.300 citações.
- Colaborações com pesquisadores de 24 países distintos.

SUMÁRIO

Preface

Professor Sylvio Canuto was born on June 6th, 1950 in Maceió/AL. He received his B.Sc. and M.Sc. degrees in Physics from the University of Brasília (UnB) and his Ph.D. in 1979 from Uppsala University, Sweden. He began his academic career as a faculty member in the Department of Physics at the Federal University of Pernambuco (UFPE), where he served from 1980 to 1994, becoming Full Professor in 1989 and Head of Department from 1989 to 1991.

In 1994, he joined the Institute of Physics of the University of São Paulo (USP), where he has served as Full Professor until 2025 and currently holds the position of Senior Professor. At USP, he was Head of the Department of Materials Physics (2004–2006) and of the Department of General Physics (2008–2012).

Professor Canuto has played a prominent role in Brazilian science administration and policy. He served as Pro-Rector for Research at the University of São Paulo from 2018 to 2022. He was a member and later President of the Physics and Astronomy Advisory Committee of CNPq (2000–2002), Coordinator of the Astronomy and Physics Area at CAPES (2011–2018). He also served as President of the Brazilian Physical Society and as General Coordinator for Sciences, Humanities, and Arts at Brazilian Agency/FAPESP.

In recognition of his scientific contributions, he was awarded the **National Order of Scientific Merit**, Commander class, in 2018. He has been a **CNPq Research Fellow**. Professor Canuto has been Co-Editor-in-Chief of *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (Elsevier) since 2016. He is a Full Member of the Brazilian Academy of Sciences (ABC), the Academy of Sciences of the State of São Paulo (ACIESP), and The World Academy of Sciences (TWAS).

He has authored approximately **300 scientific papers**, his publications involve co-authorships with collaborators from **24 different countries**, reflecting the international impact and collaborative nature of his research.

The editors apologize for the absence of many of Sylvio's friends and collaborators who would have liked to contribute to this book. We wish Sylvio a happy birthday and hope to return for his 80th birthday.

The Editors

1

GaAs clusters and Multi-electron Defects as Pillars of Semiconductors

Adalberto Fazzio[1]

1.1 INTRODUCTION

In the early 1930s, there emerged a major impetus for the scientific study of semiconductors, driven in large part by A. H. Wilson's landmark article 'The Theory of Electronic Semiconductors' [1]. At the time, companies were already seeking a replacement for vacuum tubes – an effort that ultimately led to the invention of the transistor by J. Bardeen, W. Shockley and W. Brattain [2,3]. These semiconductor materials were doped with so-called shallow impurities, whose behavior was later elegantly captured by the effective-mass theory formalized by Kohn and Luttinger [4]. Depending on the impu-

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rity, the material can exhibit n-type or p-type behavior. When impurity-induced states lie close to the conduction band, the semiconductor becomes n-type; conversely, when these states lie near the valence band, it becomes p-type. The energy spectrum of these shallow impurity states resembles that of the hydrogen atom and can be expressed as

$$E_n = -\frac{m^* e^4}{8\varepsilon^2 h^2 n^2} \tag{1.1}$$

where m^* is the effective mass of the electron (or hole), ε is the dielectric constant, and n is an integer quantum number.

These impurities can change the electrical conductivity by several orders of magnitude. For instance, replacing a silicon atom with a phosphorus atom creates an n-type material, while substitution with boron yields p-type behavior. Understanding shallow impurities was essential for the Bell Labs team in developing the first transistor.

A good description of these impurity centers is obtained when the impurity belongs to a nearby group in the periodic table relative to the host crystal. However, atoms that differ significantly from the host introduce localized states deep within the bandgap -so-called deep levels – which cannot be described by the effective-mass approximation. Theoretical studies of deep levels began in the early 1970s using semi-empirical methods such as Hückel [5] and complete neglect of differential overlap (CNDO) approaches [6,7].

However, from an experimental perspective, there already existed a wealth of data – notably summarized in Deep Impurities in Semiconductors by A. G. Milnes [8]. Later, toward the late 1980s, Green’s function techniques were introduced within the large-unit-cell framework to properly account for periodic translational symmetry.

During my doctoral research, I investigated deep impurity centers in semiconductors such as GaAs, GaP, Si, Ge, and diamond [9,10]. It was in this context that I began collaborating with my colleague and friend, Professor Canuto, who had extensive experience in Hartree-Fock-Roothaan and configuration interaction (CI) methods. Together, we published several papers on this topic. One of them, “Many-electron treatment of the off-center substitutional O in Si” (Physical Review – Rapid Communications, Ref. [11]), analyzed the so-called A-center; I will discuss its main results in Section II.

Another topic we explored concerned the idea that small atomic clusters could act as precursors of macroscopic structures. In 1985, Smalley, Kroto, and Curl discovered a new form of carbon, fullerene (C60), which generates tremendous excitement across astrophysics, chemistry, and physics. The synthesis of C60 was achieved via laser ablation, involving laser vaporization followed by supersonic expansion.

At the time, researchers recognized the studying atomic clusters was essential to understanding the transition from atomic to bulk matter. These studies concentrated mainly on group IV and III-V semiconductors, where clusters are viewed as a bridge between molecular systems and the crystalline solid state.

Interestingly, Smalley himself extended his investigations to GaAs clusters around 1995, shortly after the fullerene discovery. Experimentally, laser vaporization followed by supersonic expansion was employed to produce GaAs clusters and their positive and negative ions. Conversely, theoretical studies on larger mixed clusters remained scarce, primarily due to computational challenges arising from structural and permutational complexity introduced by multiple atomic species. As a result, only a limited number of studies on small GaAs clusters had been reported up to that time [12]. We will discuss its main results in Section III.

1.2 A-CENTER

How can we show that the pseudo-Jahn-Teller (PJT) effect is responsible for the formation of the A-center? The strategy was to consider a method that allows us to quantify the interaction of configurations involving the ground state and the excited states. We adopt the cluster-approach with hydrogen-saturation boundary conditions, and the electronic structure is obtained using the INDO/1-CI method. This semi-empirical self-consistent Hartree Fock (SCF-HF) scheme, based on a linear combination of atomic orbitals (LCAO) expansion and including one-center exchange integrals, is particularly suited for