ChemPhysChem

Cover Profile
doi.org/10.1002/cphc.202100567

Chemistry Europe
European Chemical Societies Publishing

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The Drude-Smith Equation and Related Equations for the Frequency-Dependent Electrical Conductivity of Materials: Insight from a Memory Function Formalism

Rudolph A. Marcus

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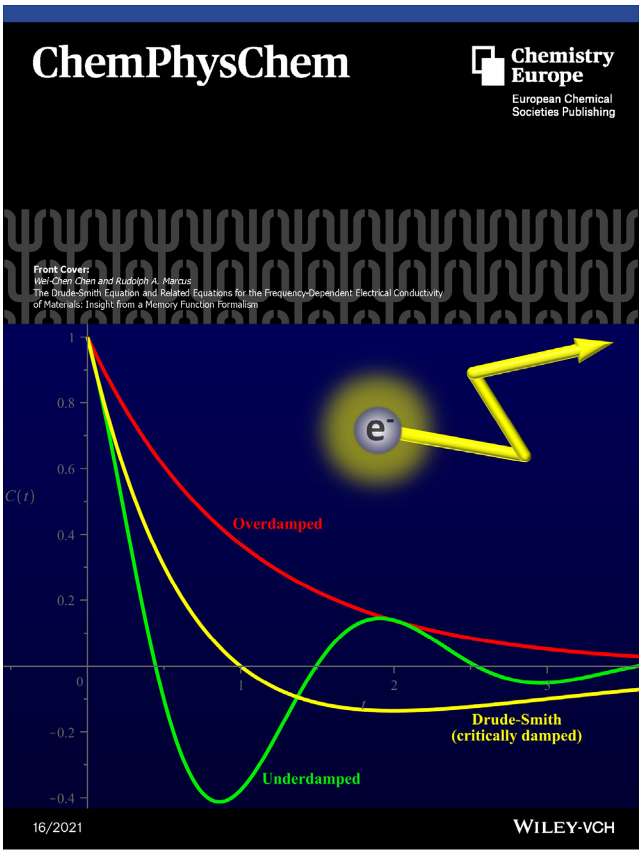
The front cover artwork is provided by Wei-Chen Chen and Rudolph A. Marcus. The image shows an electron undergoing backscattering in a disordered solid, a phenomenon commonly described using the Drude-Smith equation represented by the damping curve. Read the full text of the Article at 10.1002/cphc.202100299.

About the authors

Dr. Wei-Chen Chen, born in Taiwan in 1976, received his BS (majoring in chemistry and minoring in physics) and his MS degrees from National Tsing Hua University. For his Ph.D. he joined Rudy Marcus' group at Caltech, where he did research in theoretical chemistry in a variety of fields ranging from atmospheric chemistry to the fluorescent behavior of dyes undergoing electron transfer on surfaces. The awards he received include the Research Creativity Award from National Science Council at Taiwan, Honorary Member of the Phi Tau Phi Scholastic Honor Society, Bray Fellowship at California Institute of Technology, and Bayer Sciences & Education Foundation Fellow. He later joined the company of Goldman Sachs in New York City, where he is now a vice president in model risk management, applying theories and mathematics not too dissimilar from those in non-equilibrium statistical mechanics, the topic that he studied in this article on the THz conductivity of somewhat disordered materials.

Rudolph A. Marcus, John G. Kirkwood and Arthur A. Noyes Professor of Chemistry at Caltech, was born in Montreal, Canada in 1923. After receiving a B.Sc. and Ph.D. from McGill University (experiments on chemical reaction rates in liquids), and post-doctoral research at the N.R.C. of Canada (experiments on chemical reaction rates in gases) and the University of North Carolina (reaction rate theory), he joined the faculty of the Polytechnic Institute of Brooklyn, the University of Illinois, and Caltech. His research includes the "Marcus theory" of electron transfer processes, the RRKM theory of unimolecular reactions, and more recent theories in fields that include anomalous isotope effects in stratospheric ozone, catalysis of 'on water' organic reactions, single molecule behavior of biological motors, and single molecule studies of molecular conductance. A trademark of his research has been a strong interaction between theory and experiment. Marcus received the Wolf Prize in Chemistry in 1985, the U.S. National Medal of Science in 1989, and the Nobel Prize in Chemistry in 1992.



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Origin of present article in ChemPhysChem

This research ultimately had its origin in the appointment of Marcus as Visiting Nanyang Professor at Nanyang Technological University by President Bertil Anderssn, where he joined the group of Professor Maria-Elisabeth Michel-Beyerle, Professor of Physics at NTU and Emerita Professor of Chemistry at the Technical University Munich. The experiments included the photogeneration of charge carriers in various materials, such as perovskite films. One of the methods applied was terahertz spectroscopy (directed by Professor E. E. M. Chia, also in NTU's Physics Department) which provided data on the frequency-dependent electrical conductivity of those films. THZ spectroscopy gave information on the number density and mobility of the charged carriers. The theory frequently used to treat the frequency-dependent electrical conductivity is the Drude-Smith theory, where in 2001 Smith added back-scattering to the theory developed a century earlier by Drude. An attractive feature of the theory is the sparsity of parameters, only two. And yet misgivings were often voiced in the literature, including that by Smith himself, because of the seeming arbitrariness of one of the steps in the derivation. The present authors recalled the numerous computational studies on back scattering in fluids and applied the memory function approach used there to place the Drude-Smith and another equation in a more general context, with the capability of suggesting extensions.

Acknowledgements

The authors are pleased to acknowledge the helpful comments and suggestions of the reviewers.

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