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# **Comprehensive Computational Chemistry**

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Comprehensive Computational Chemistry는 해당 분야의 전체적인 내용을 다루는 150개 이상의 챕터로 구성되어 있습니다. 기본 원리를 다루는 이론적 방법, 알고리즘, 소프트웨어 패키지 개발, 대기화학, 생화학, 재료과학, 의학 등 다양한 분야의 광범위한 응용 방법에 대해 탐구합니다. 세계적으로 유명한 과학자 팀이 편집하였으며 양자 화학의 이론적 기초부터 화학 반응 모델링의 복잡성, 분자 시스템의 역학을 탐구하며 여러 응용 분야에서의 촉매를 이해하고 설계하는 데 있어 계산 화학의 중요한 역할을 다루고 있습니다. 이 분야의 입문자, 연구자, 학생 등 끊임없이 발전하는 계산 화학을 알아가는 데 있어 필수적인 자료입니다.





# Meet the editors

Editor-in-Chief

#### Russell J. Boyd

Russell J. Boyd is Alexander McLeod Professor Emeritus at Dalhousie University. He graduated in 1967 with First-Class Honours and the Gold Medal in Chemistry from the University of British Columbia and upon receiving his PhD in 1971 in theoretical chemistry from McGill University, he went to Oxford University as an NRC postdoctoral fellow with Charles Coulson at the Mathematical Institute. In 2001 he became the seventh Alexander McLeod Professor of chemistry. He has published around 300 peer-reviewed papers and review chapters in computational and theoretical chemistry and is a member of the Scientific Board of the World Association of Theoretical and Computational Chemists and Chair of WATOC 2020. His awards include the fellowship and 2009 Montreal Medal of the Chemical Institute of Canada in recognition of his distinguished contributions to the profession of chemistry in Canada. His many professional activities include serving as editor for theoretical chemistry for 2007–08, and chair of The Chemical Institute of Canada for 2012–13. He was elected to the Bureau of the International Union of Pure and Applied Chemistry in 2013 and acted as the Section Editor for the Theoretical and Computational Chemistry section of the Elsevier Reference Module in Chemistry and Chemical Engineering.

#### Manuel Yanez

Manuel Yáñez got his B.Sc. in Chemistry (1st class honours) in 1970 at the Universidad de Santiago de Compostela in 1970 and his PhD (Special Prize to the best PhD. Thesis) at the Universidad Autónoma de Madrid in 1973.He was postdoc with John Pople (Noble Laureate in 1998) from 1974 to 1976 at Carnegie-Mellon University. Back in Spain he got in 1979 a tenure as Associate Professor and in 1983 as Full Professor of Physical Chemistry at the Universidad Autónoma de Madrid. He received several research awards, among them, the Award of the UAM Foundation in 1993, the Research award in Physical Chemistry of the Royal Spanish Society of Chemistry in 2001, the Bettancourt-Perronet Award from the Ministry of Education and Research of France in 2003 and the Award for a Distinguished Career from the Royal Spanish Society of Chemistry in 2018. He was appointed Academician of the Royal Academy of Exact, Physical and Natural Sciences (RACE) and was invested Doctor Honoris Causa by the University of the Basque Country. He was the Coordinator of a European Erasmus+ Master and of a European Joint Doctorate on Theoretical Chemistry and Computational Modelling. He is author of more than 500 papers and several book chapters as well as having been a long-standing co-Editor in Chief of the successful Elsevier Journal, Computational and Theoretical Chemistry and Editor in Chief of Anales de Química of the Spanish Royal Society of Chemistry (RSEQ).

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