



André Mischke YAE Prize for Science and Policy

Laudator



TITLE AND FULL NAME: Professor Marcel Swart

AFFILIATION: ICREA; IQCC (Univ. Girona); Young Academy of Europe

LINK TO WEBPAGE: www.marcelswart.eu

BIOGRAPHICAL NOTE

Marcel Swart obtained his PhD in theoretical chemistry at the University of Groningen (NL) with a study on copper proteins (2002). He works since 2006 at the IQCC (Univ. Girona), and was promoted to ICREA Research Professor in 2009. He has published ca. 140 papers, formed part of tribunals for Masters and PhD ceremonies, evaluation committees (ANEP, FWO, La Caixa), reviewer for >40 journals and (inter)national science organizations. He received funding from science organizations and companies, organized a CECAM/ESF Workshop (Zaragoza, 2012) and was the main organizer of Girona Seminars (2016, 2018). He is Editor of a Wiley-book on "Spin states in Biochemistry and Inorganic Chemistry" (2015), director IQCC, Outgoing Chair of the Young Academy of Europe, and was Chair of COST Action CM1305 (ECOSTBio). He supervised five PhD theses (two with Premi Extraordinari), was awarded the Young Scientist Excellence Award 2005, MGMS Silver Jubilee Prize 2012, was elected Fellow of the Young Academy of Europe (2014), Fellow of Royal Society of Chemistry (2015) and Member of Academia Europaea (2019).

He works in the field of theoretical (bio)inorganic and supramolecular chemistry, and works on transition-metal complexes, metalloproteins, enzymes, and DNA. The effect of (transition) metal ions on reactivity, selectivity and chemical bonding is one of the main topics in these studies. The development of computational tools for these studies is an important ingredient, to which he has contributed largely both with his own software (QUILD, DRF90) as in contributions in general purpose software (ADF, NWCHEM). One of the main areas where these tools are applied is in the field of transition-metal chemistry, the spin states involved, and the effect this has on reactivity. For this he developed spin-state consistent density functionals (SSB-D, S12g).