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His scientific background includes physical chemistry, catalysis, quantum chemistry, atomistic methods, programming languages, operating systems, and parallel computing. He has been user of large computational facilities across Europe.

His main interest is focused on physico-chemical properties of materials in the solid state using all kinds of computational tools, where he has published over 100 papers in topics such as: molecular mechanics, molecular dynamics, atomistic forcefields, quantum chemistry, ab-initio methods, and density functional theory.

