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Preface

Some thirty-five years have passed since I first contacted Per-Olov Löwdin about the possibility of getting a job related to numerical computations at Uppsala. What I expected to be a part time occupation to support me through graduate school proved to be a total experience where I was immersed in a sea of unfathomable depth and had to learn the strokes of swimming or timidly drown in the waves of quantum theory. Per-Olov Löwdin conveyed the enthusiasm, the dedication, and the discipline of work which are so essential in any endeavour but possibly most acutely needed in the pursuit of scholarly and artistic accomplishment. I am proud to be the guest editor of an issue of this journal where Per-Olov Löwdin's achievements are celebrated and to have this opportunity to express my gratitude for the continuing inspiration he provides.

The editorial prerogative allowed me to select as a theme for this issue the three papers which Per-Olov Löwdin published in the Physical Review in 1955, to some known as his revelations. These have in a particular fashion shown their lasting value and the concepts which were introduced there are now part of the repertoire in the theory of molecular electronic structure or, nearly equivalently, quantum chemistry. Löwdin's numerical work on ionic crystals and his ingenious treatment of the overlap problems had given him the experience in data management that allowed him to see and extricate the general structure of many-electron wave functions, basis set methods, superposition of configurations, density matrices, natural orbitals, and generalized variational procedures. These were hot topics at the Quantum Chemistry Group at Uppsala in the mid to late fifties and Per-Olov Löwdin's early morning lectures gave the audience the very best of introductions to his effective and economical formulations of quantum theory. The many hours of individual studies of the papers have been amply rewarded over the years. One acquired a resource of formalisms and theoretical structures which permitted a necessary stratification of the scientific literature and provided the important appreciation of the historical relations between current efforts and the existing body of knowledge. Per-Olov Löwdin insists on the most direct and clear presentation of theory. He often describes the scientific quest as finding paths over challenging mountain passes to pastures of conceptual beauty. The first route may be obtained by erratic penetrations of thorny thickets, but the goal is to find a clean, albeit demanding passage through "chimneys" or across icy glaciers.

An ever growing number of quantum chemists are being educated in terms of concepts which were detailed and formulated in Per-Olov Löwdin's 1955 papers in The Physical Review. The contributors to this volume are paying homage to Löwdin and his "economy-of-thought" approach to theory by utilizing the concepts of natural orbitals, reduced density matrices, electron densities, and projection operators in their contemporary presentations. Treatments of the electron correlation through extended use of superposition of

configurations is the order of the day and only a rational application of the means of analysis introduced by Löwdin can give a conceptual content to such investigations. The natural orbitals have assumed a position of significance which was anticipated by him through some early studies and they have come to the fore in recent times in the advanced design of basis sets. Density functional theory has assumed an ever growing place in solid state theory and quantum chemistry and although Per-Olov Löwdin never embraced this formalism he did contribute, in the 1955 series, to its development with an original variational form for the determination of the effective one-electron potential. He was convinced that the use of extended basis sets and optimization procedures such as they are seen in multiconfigurational approaches would prevail and that the natural orbital contractions provide the necessary means for compacting the result. The current state of affairs has borne him out. Per-Olov Löwdin has a special relation to nonorthogonal sets of basis functions and it is particularly pertinent in this issue to see a contribution in the valence-bond formulation where overlap is a most important issue. The formal development of new concepts, continuing Löwdin's efforts, is well represented among the contributors to this issue and I am pleased to submit the collection to the literature as a fitting tribute to a great scientist and an outstanding scholar.

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