

Preface

A new century of theoretical chemistry

The end of the century provides a time to look back, and the start of a new century inspires one to look ahead. For this New Century Issue of *Theoretical Chemistry Accounts*, we asked the advisory editors of the journal to identify a paper from the first century of theoretical chemistry and discuss its importance for the twentieth century with an eye towards the twenty-first century. Although we collected 66 such perspectives, they are far from representing a full set of the papers deserving our reflection. At one point we thought of inviting additional perspectives to fill some obvious gaps or provide better balance, but we decided that any such attempt would spoil the spontaneity of the collection, which is part of its interest.

We hope the *Theoretical Chemistry Accounts* New Century Issue will be entertaining, but even more we hope it will help younger scientists to see the role that selected creative efforts of the past have played in getting us to the present. Further, to the extent that this issue inspires members of the theoretical chemistry community to reread the papers that led to the present state of the art, that is all to the good, because there is still a lot to be learned from the last century's literature. Finally, taking this issue as prolog, we can all try to make our upcoming efforts as influential for the next century as these papers were for the last.

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December 31, 1999