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Molecular Quantum Mechanics in the Born–Oppenheimer Limit

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Abstract. Born–Oppenheimer approximations describe molecular quantum mechanics in the limit of large nuclear masses. Although these approximations are almost eighty years old and fundamental to theoretical chemistry, their rigorous mathematical analysis began only thirty years ago. Most of this analysis has concentrated on validating existing physical theories, but some has led to new insights concerning molecular dynamics.

We review the mathematical work in this subject and describe some directions in which we hope some future progress might be made.