# Recent progress on accurate *ab initio*-based potentials and dynamics: atmospheric $N_xO_y$ triatomic systems and beyond

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The talk starts by addressing the "road-map" of theoretical chemical physics: the Born-Oppenheimer-Huang (BOH) approximation[1]. Specific issues are next considered covering electronic structure and dynamics studies of oxygen atoms, nitrogen atoms, oxygen molecules, and nitrogen molecules in the gas phase. First, a cost-effective *ab initio* scheme to generate accurate potentials[2] is presented. Second, their representation via double many-body expansion theory is considered, with illustrations given for[3-6] $N_3$, $N_2O$ and $NO_2$. Multi-sheeted potential forms[4,6] will then be also discussed, and past work and planned activity on the relevant tetratomic potentials using density functional theory approaches with the Minnesota density functionals[7] briefly outlined. Additionally, cross sections, rate constants and non-adiabatic effects obtained by running trajectories on the above potentials are presented. Serving for validation purposes, such results will also be utilized in future work for understanding key physical processes in high-temperature hypersonic flows and help on developing accurate and validated thermochemical models and associated rate data for use in flow simulations.

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## References

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