Supporting Information of "Excited States From State Specific Orbital Optimized Pair Coupled Cluster"

Fábris Kossoski,[1, a)] Antoine Marie,[1] Anthony Scemama,[1] Michel Caffarel,[1] and Pierre-François Loos[1, b)]

Laboratoire de Chimie et Physique Quantiques (UMR 5626), Université de Toulouse, CNRS, UPS, France

[a)]Electronic mail: fkossoski@irsamc.ups-tlse.fr

[b)]Electronic mail: loos@irsamc.ups-tlse.fr

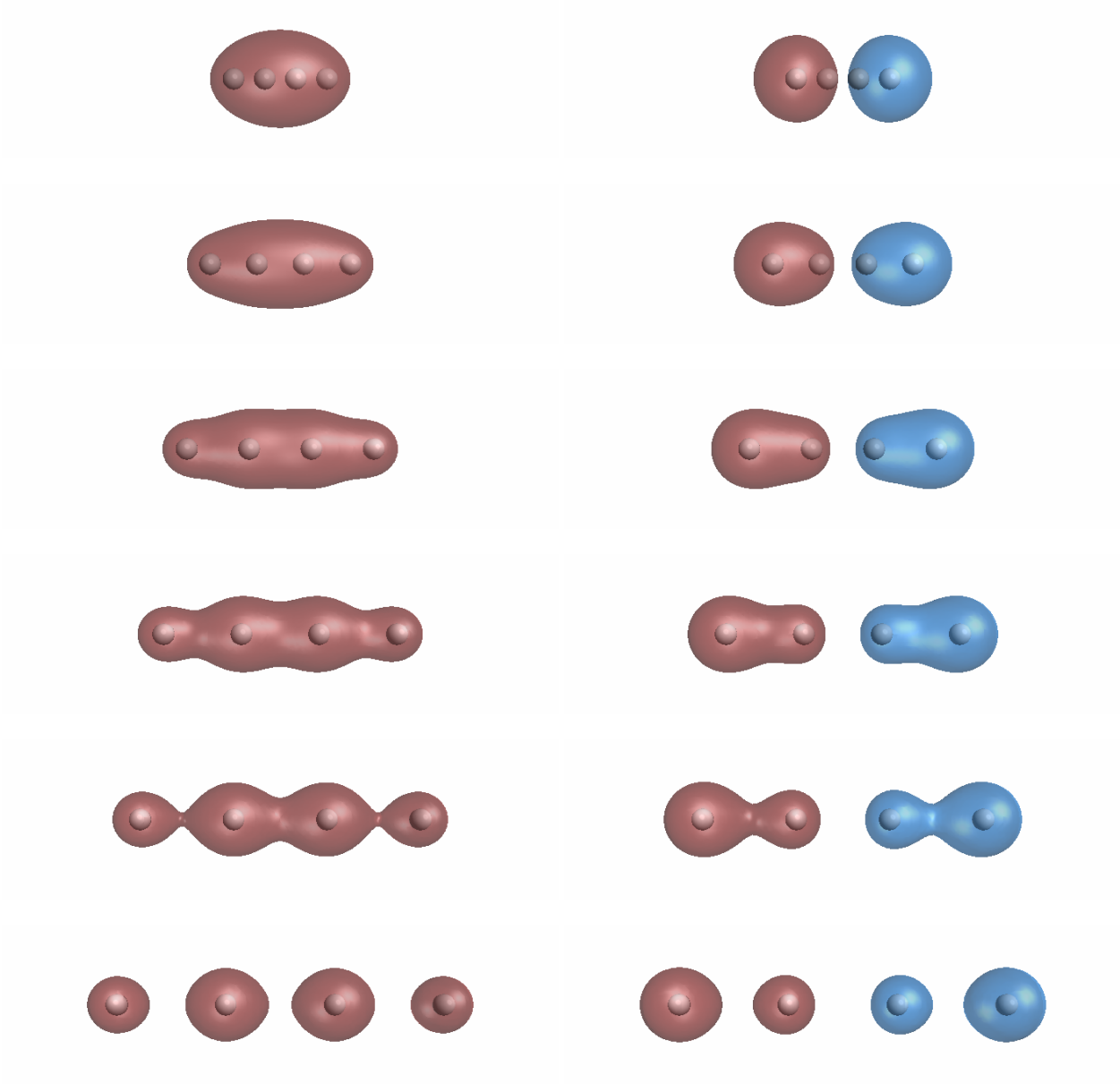

FIG. 1. Canonical Hartree-Fock orbitals for the ground state $[(\sigma_g)^2(\sigma_u)^2]$ of linear H_4, computed from $R_{H-H} = 1a_0$ up to $R_{H-H} = 3.5a_0$, in steps of $0.5a_0$, from top to bottom.

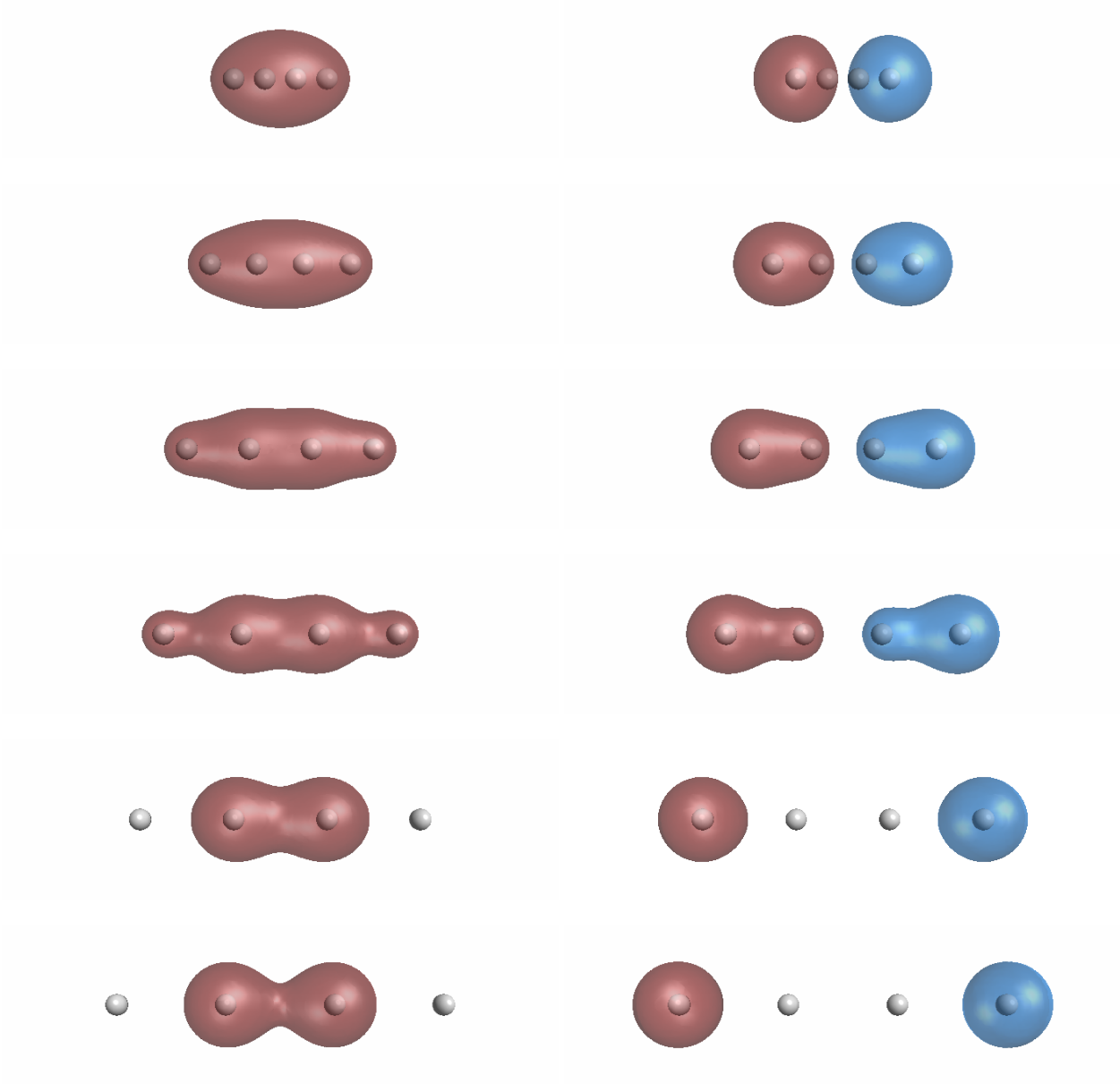

FIG. 2. Variationally optimized orbitals at the pCCD level, for the ground state $[(\sigma_g)^2(\sigma_u)^2]$ of linear H_4, computed from $R_{H-H} = 1a_0$ up to $R_{H-H} = 3.5a_0$, in steps of $0.5a_0$, from top to bottom.

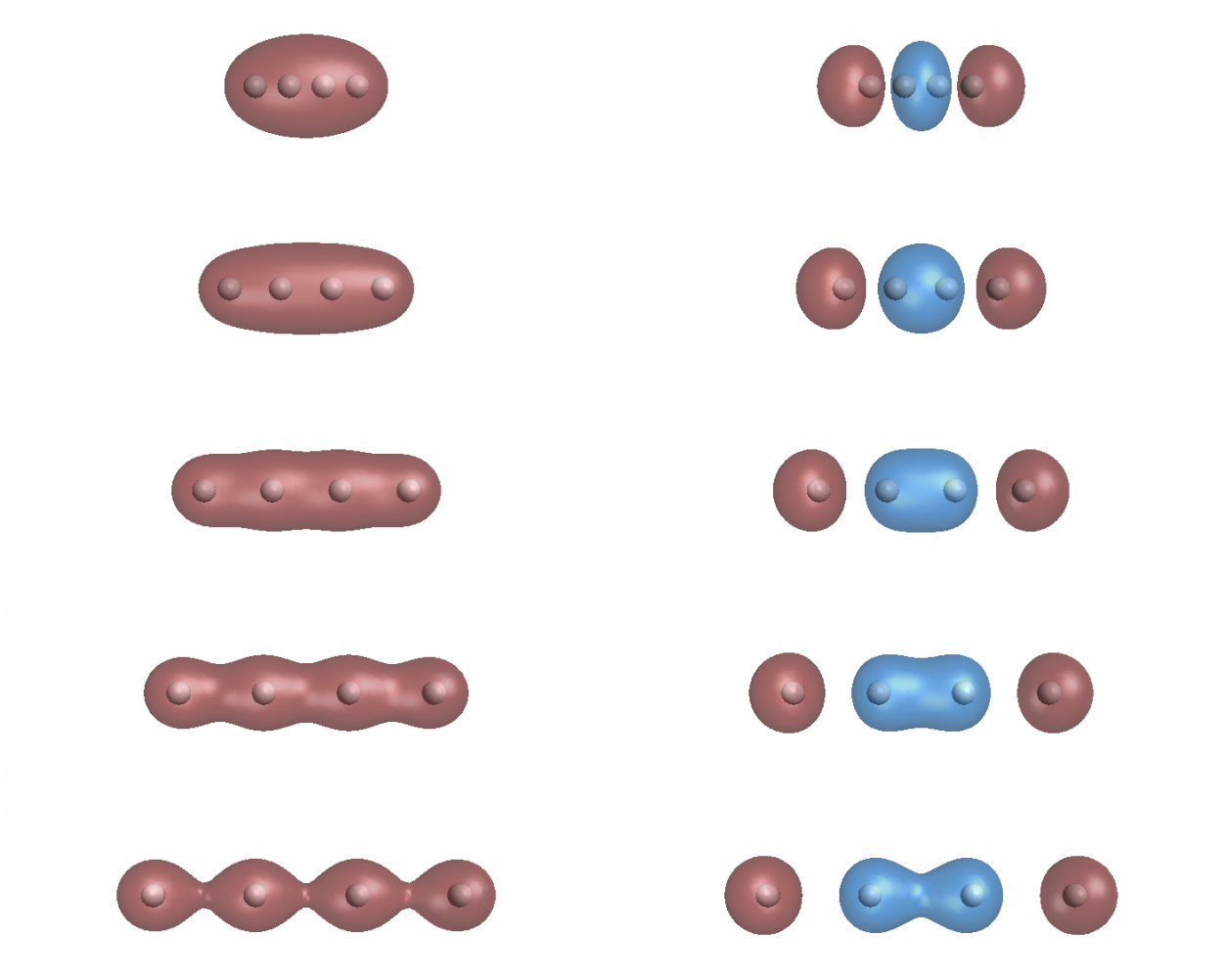

FIG. 3. Variationally optimized orbitals at the pCCD level, for the first doubly-excited state $[(\sigma_g)^2(\sigma_g^*)^2]$ of linear H_4, computed from $R_{H-H} = 1a_0$ up to $R_{H-H} = 3.5a_0$, in steps of $0.5a_0$, from top to bottom.

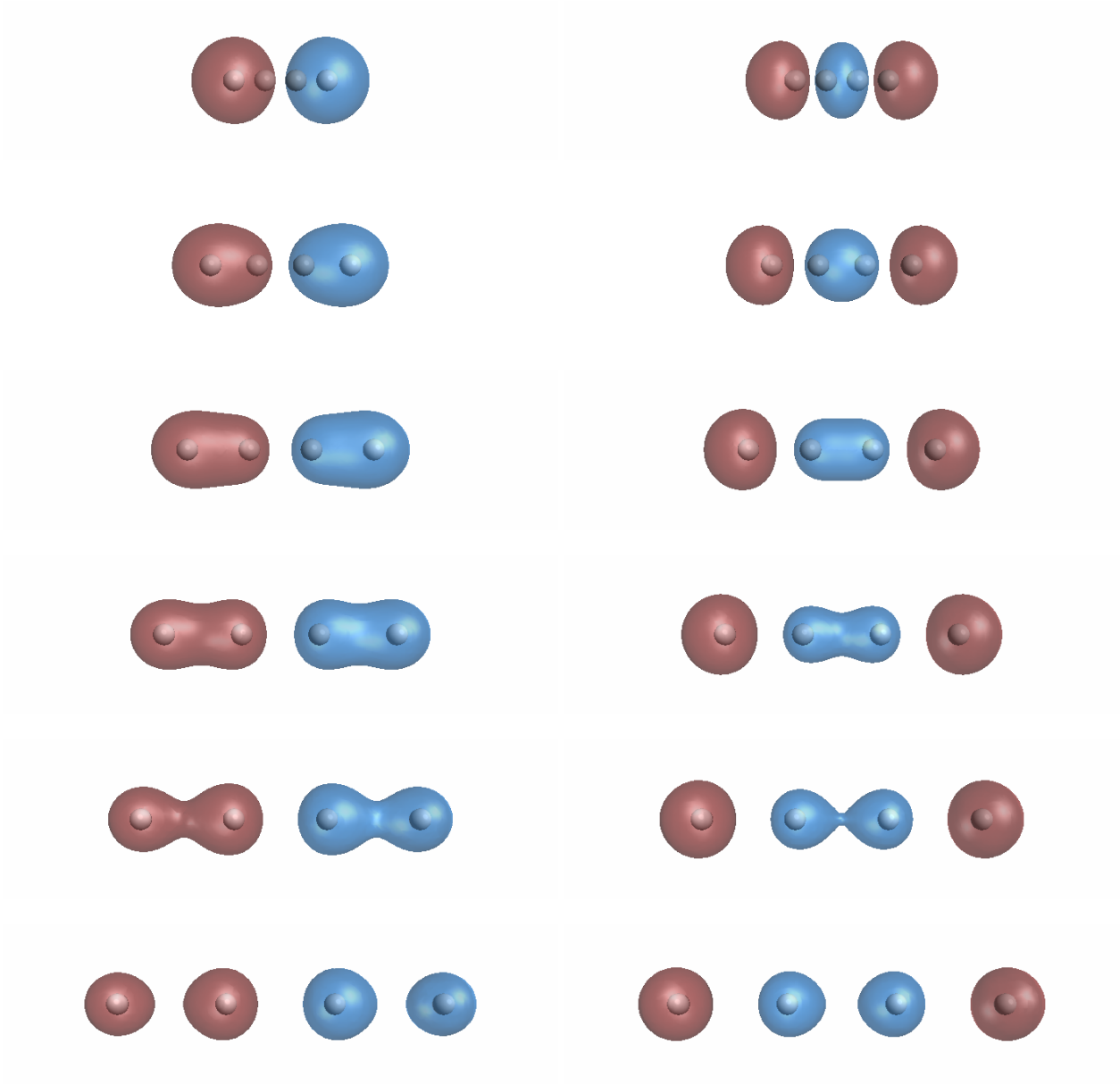

FIG. 4. Variationally optimized orbitals at the pCCD level, for the second doubly-excited state $[(\sigma_u)^2(\sigma_g^*)^2]$ of linear H_4, computed from $R_{H-H} = 1a_0$ up to $R_{H-H} = 3.0a_0$, in steps of $0.5a_0$, from top to bottom.

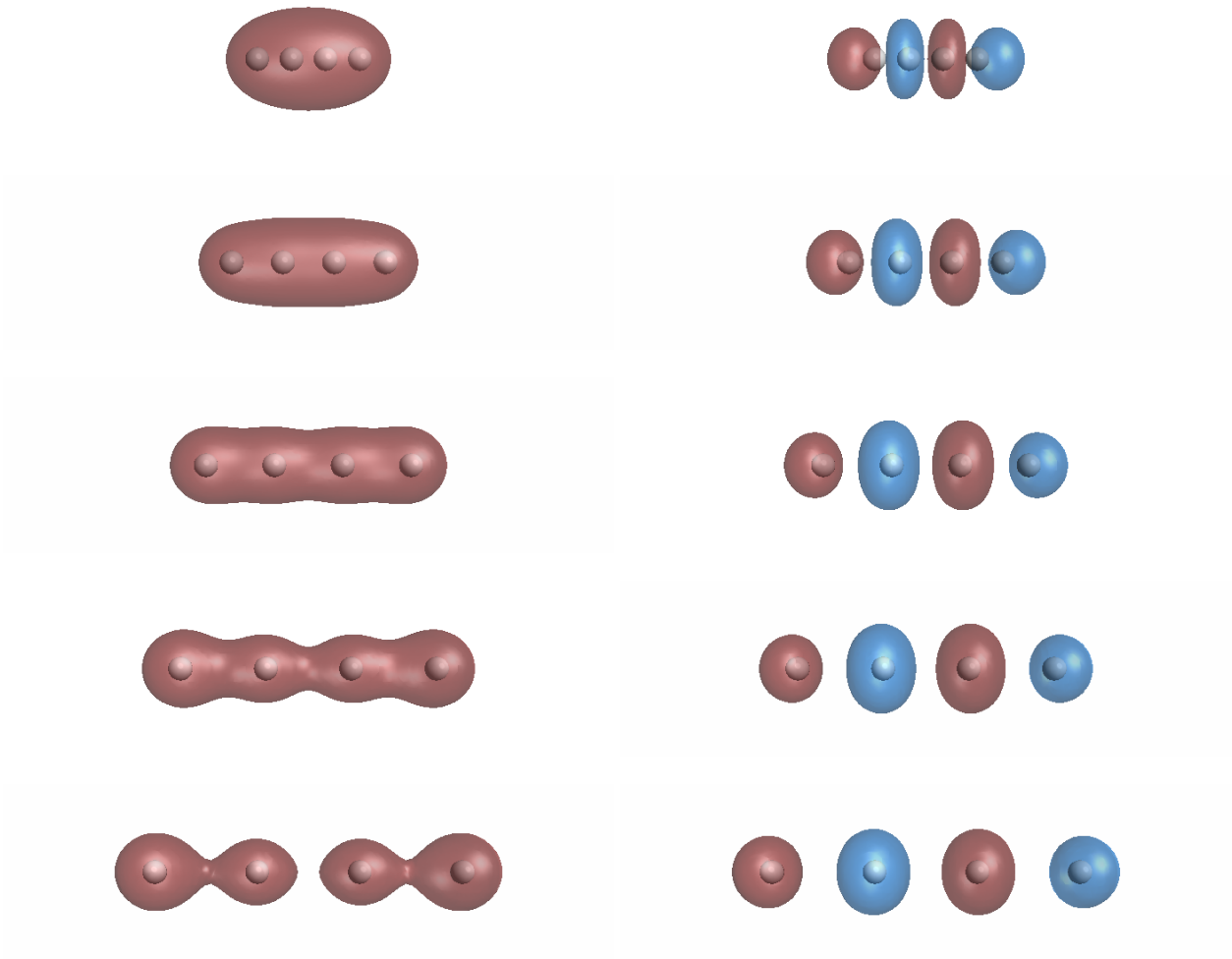

FIG. 5. Variationally optimized orbitals at the pCCD level, for the third doubly-excited state $[(\sigma_g)^2(\sigma_u^*)^2]$ of linear H_4, computed from $R_{H-H} = 1a_0$ up to $R_{H-H} = 3.5a_0$, in steps of $0.5a_0$, from top to bottom.

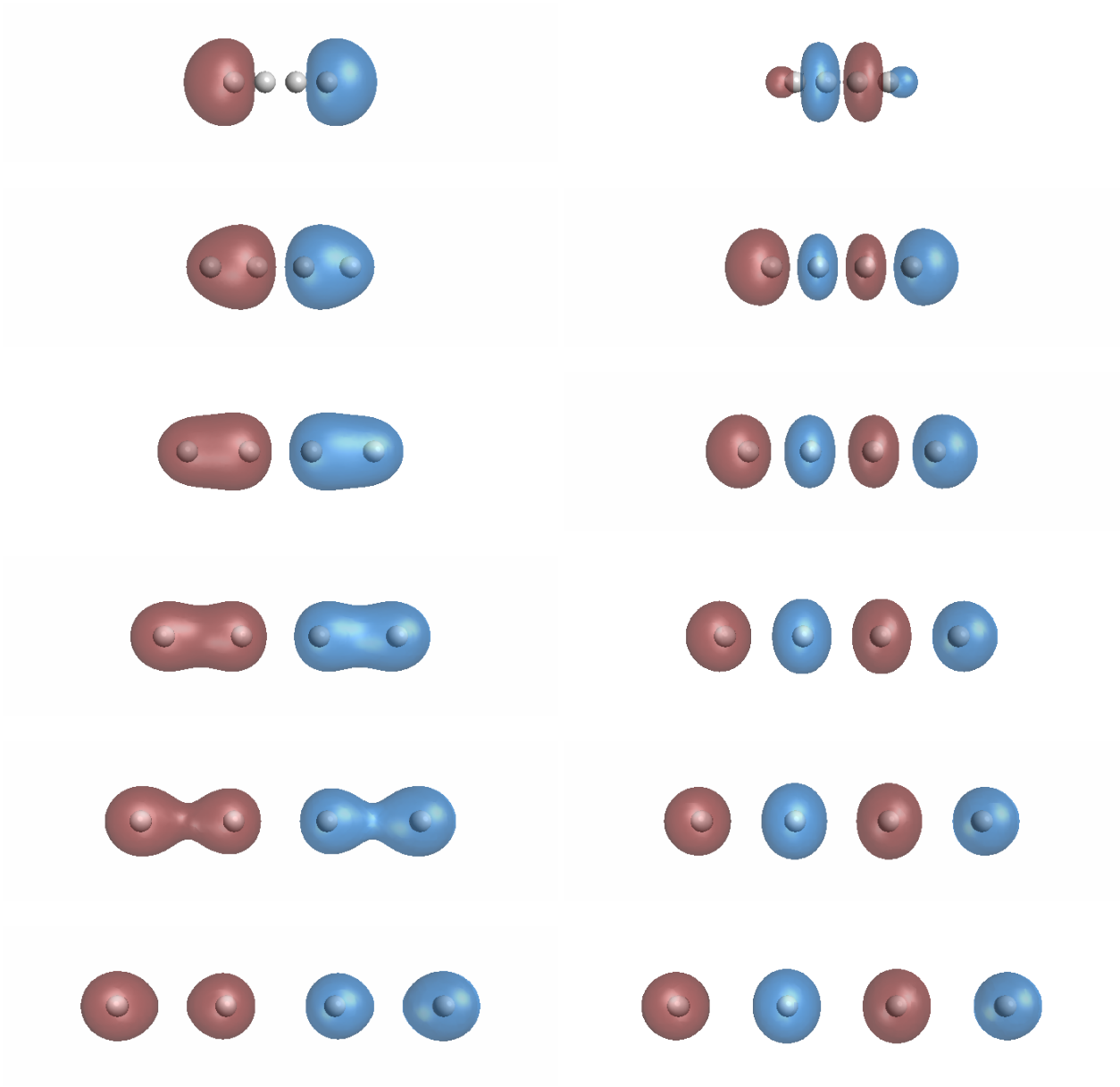

FIG. 6. Variationally optimized orbitals at the pCCD level, for the fourth doubly-excited state $[(\sigma_u)^2(\sigma_u^*)^2]$ of linear H_4, computed from $R_{H-H} = 1a_0$ up to $R_{H-H} = 3.5a_0$, in steps of $0.5a_0$, from top to bottom.

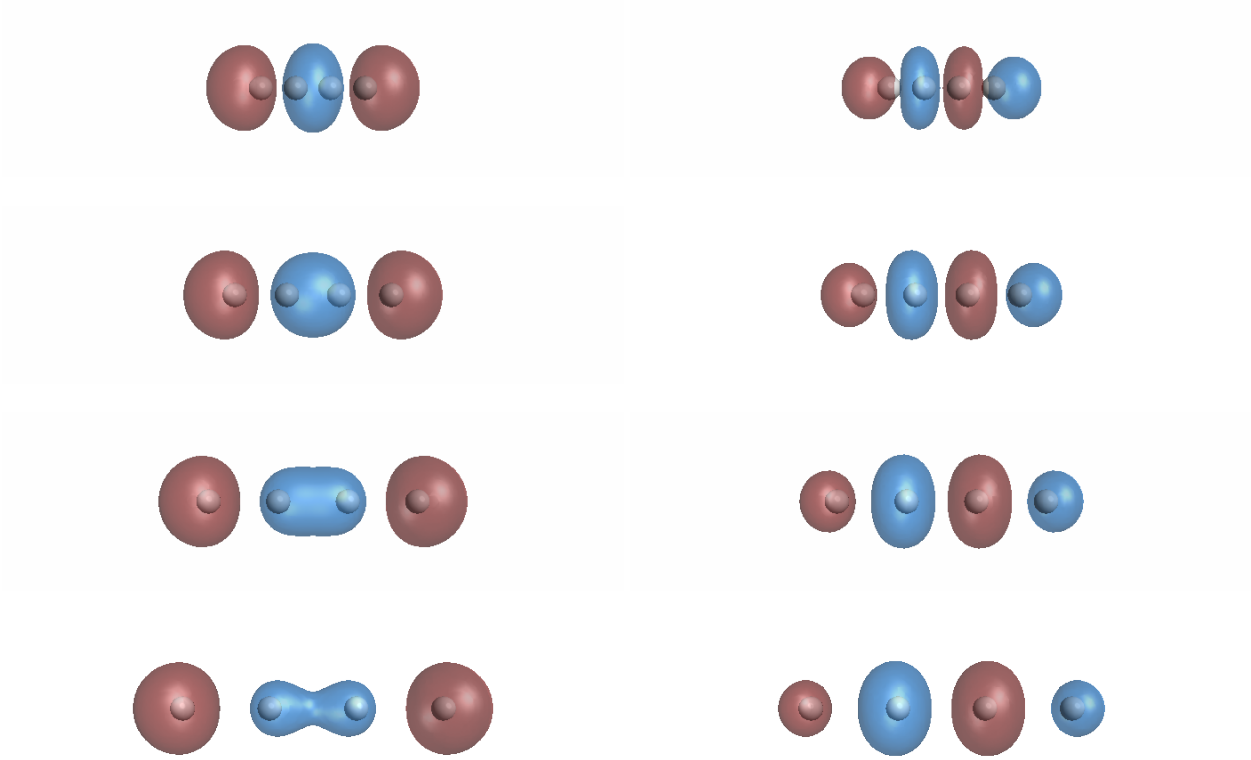

FIG. 7. Variationally optimized orbitals at the pCCD level, for the fifth doubly-excited state $[(\sigma_g^*)^2(\sigma_u^*)^2]$ of linear H_4, computed from $R_{H-H} = 1a_0$ up to $R_{H-H} = 3.5a_0$, in steps of $0.5a_0$, from top to bottom.

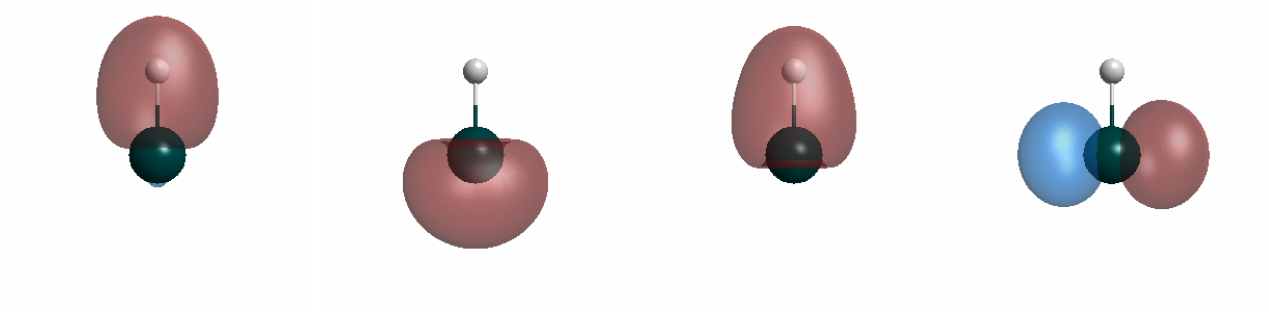

FIG. 8. Variationally optimized orbitals at the pCCD level, for the ground (two leftmost) and the doubly-excited (two rightmost) states of BH.

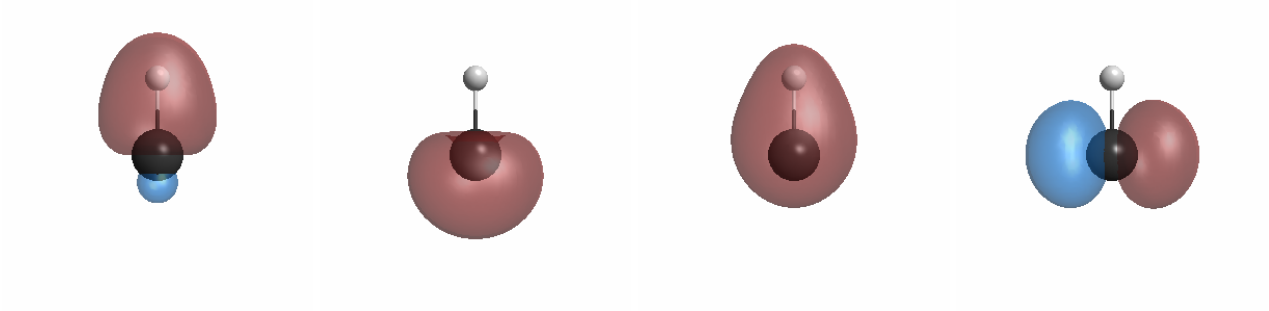

FIG. 9. Variationally optimized orbitals at the pCCD level, for the ground (two leftmost) and the doubly-excited (two rightmost) states of CH^+.

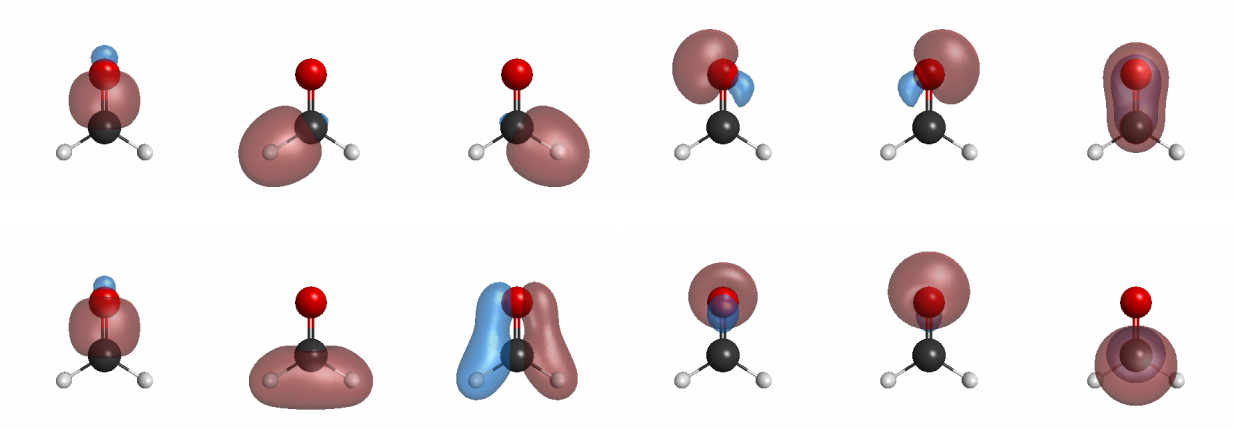

FIG. 10. Variationally optimized orbitals at the pCCD level, for the ground (top row) and the doubly-excited (bottom row) states of formaldehyde.

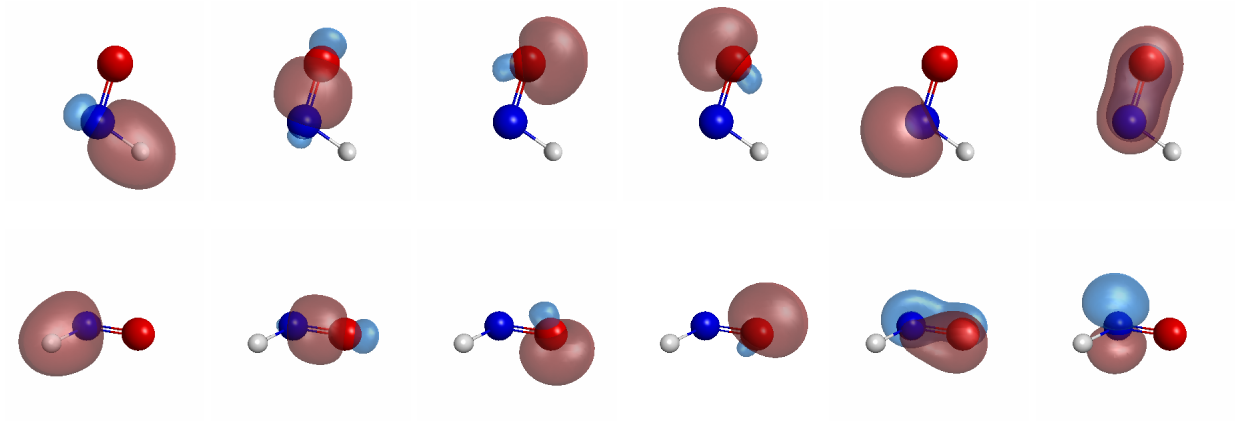

FIG. 11. Variationally optimized orbitals at the pCCD level, for the ground (top row) and the doubly-excited (bottom row) states of nitroxyl.

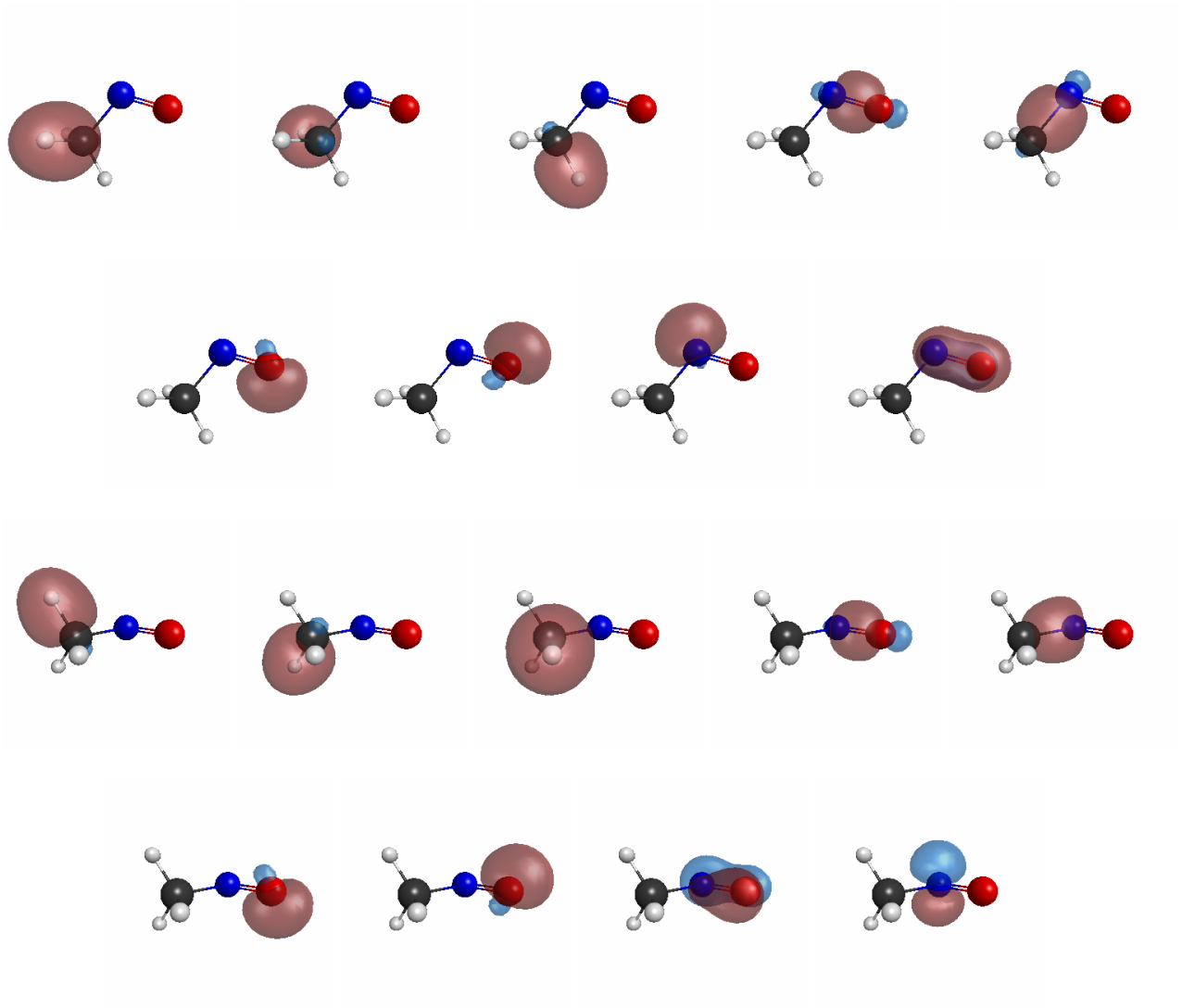

FIG. 12. Variationally optimized orbitals at the pCCD level, for the ground (top two rows) and the doubly-excited (bottom two rows) states of nitrosomethane.