Supporting Information: Perturbation of the UV transitions of formaldehyde by TiO_2 photocatalysts and Au_n nanoclusters

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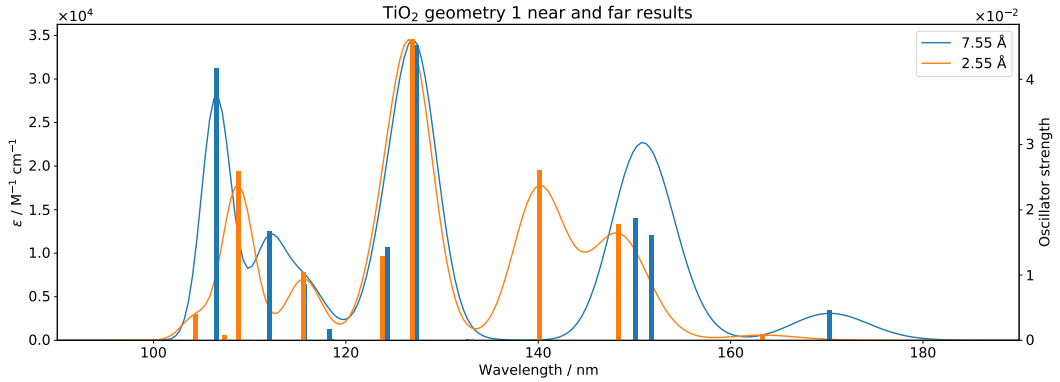
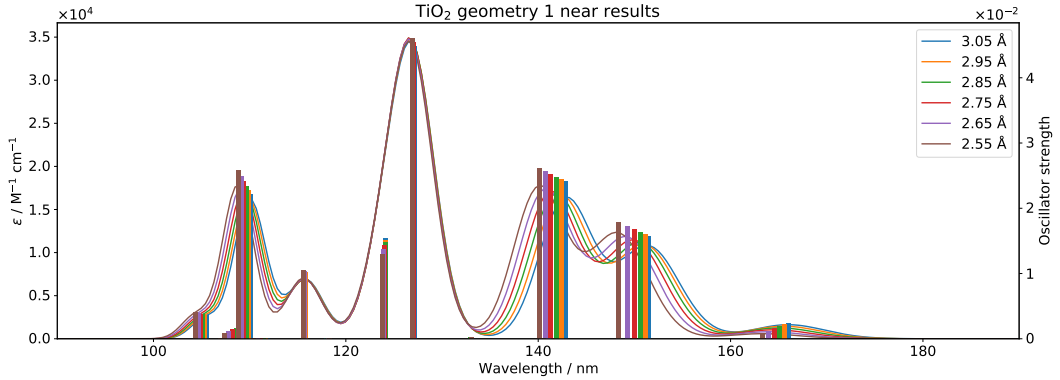
1 UV-Vis spectra for formaldehyde on TiO_2

Calculated UV-Vis spectra of formaldehyde when placed on the TiO_2-surface. All excitation energies and oscillator strengths have been calculated with the CCSD linear response method and the aug-cc-pcTZ basis set. For each geometry the difference in the UV-VIS spectra between the closest and farthest position of formaldehyde (near and far results) and the change in the spectra when formaldehyde is in the six closest positions (near results).

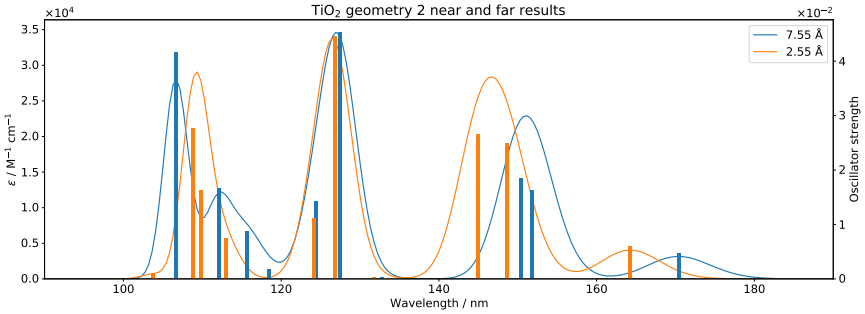


(a) UV-VIS: Formaldehyde in geometry 1. Nearest and farthest distance

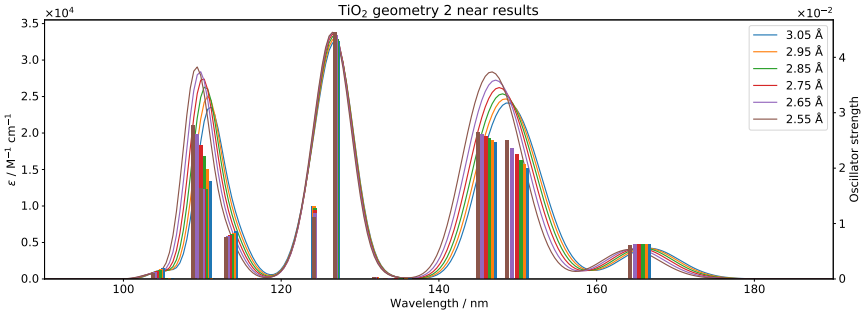


(b) UV-VIS: Formaldehyde in geometry 1. The six nearest distances

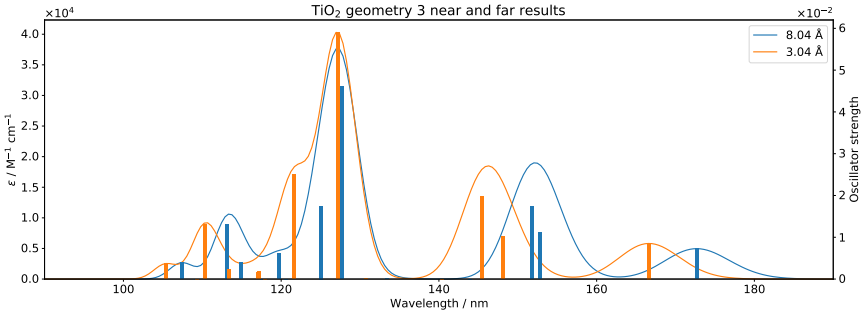
Figure 1: Results for TiO_2 geometry 1



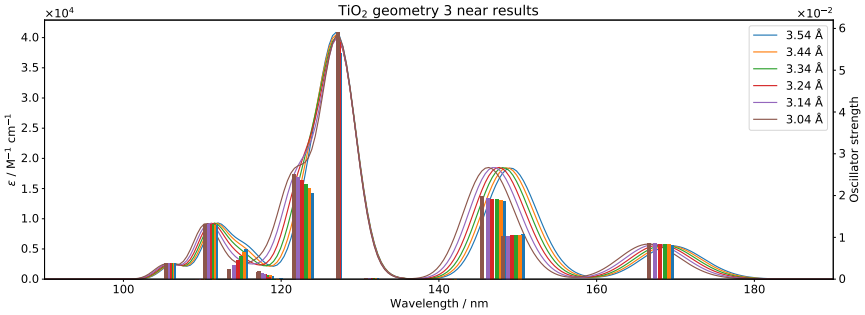
(a) UV-VIS: Formaldehyde in geometry 2. Nearest and farthest distance



(b) UV-VIS: Formaldehyde in geometry 2. The six nearest distances

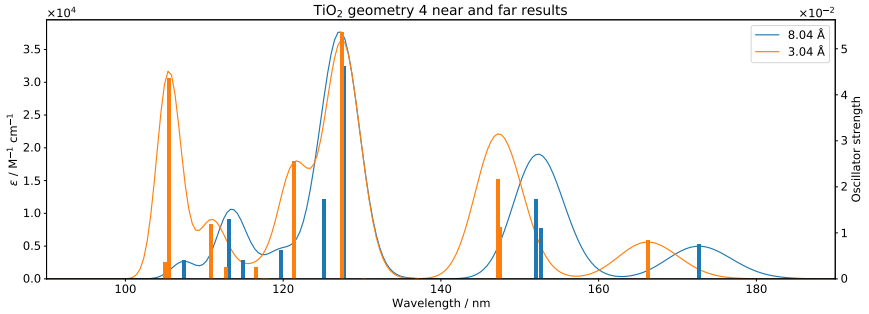


(c) UV-VIS: Formaldehyde in geometry 3. Nearest and farthest distance

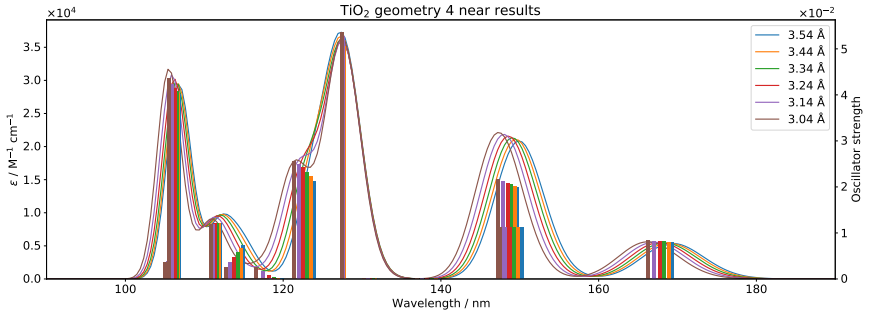


(d) UV-VIS: Formaldehyde in geometry 3. The six nearest distances

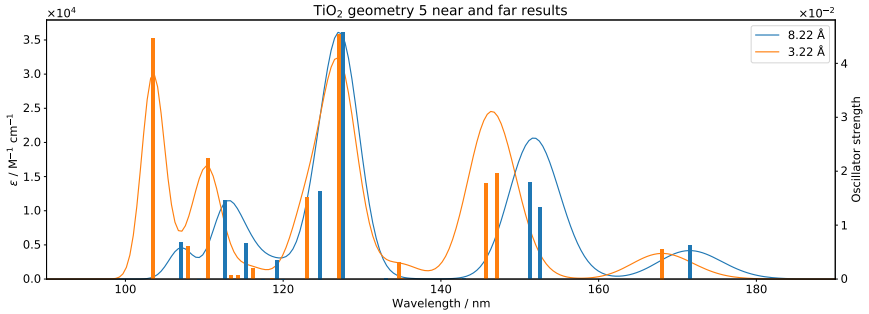
Figure 2: Results for TiO_2 geometry 2 and 3



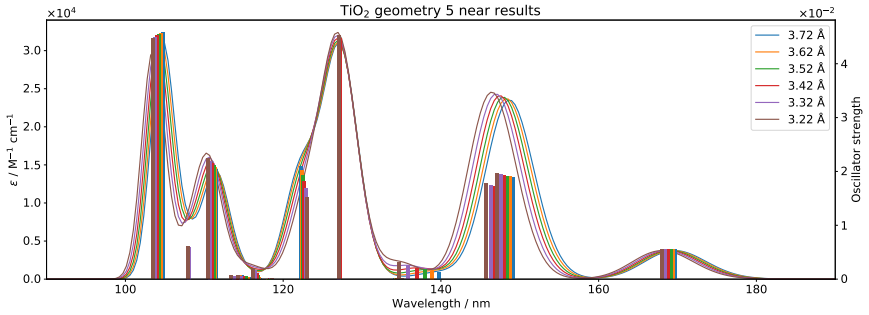
(a) UV-VIS: Formaldehyde in geometry 4. Nearest and farthest distance



(b) UV-VIS: Formaldehyde in geometry 4. The six nearest distances

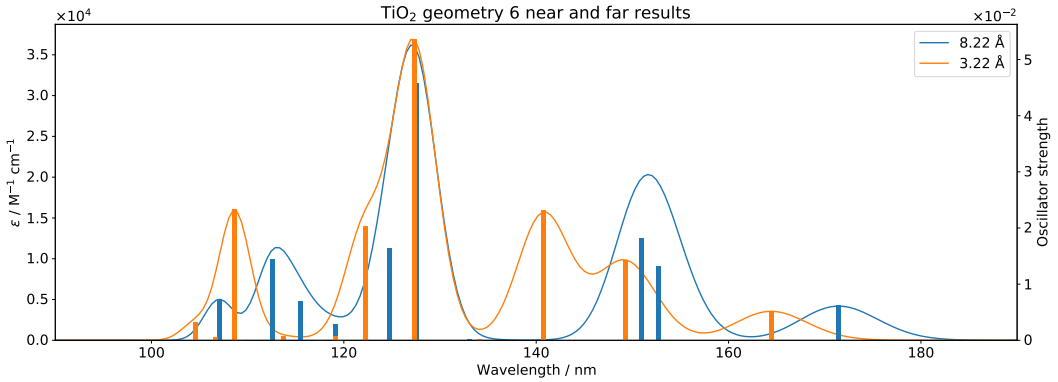


(c) UV-VIS: Formaldehyde in geometry 5. Nearest and farthest distance

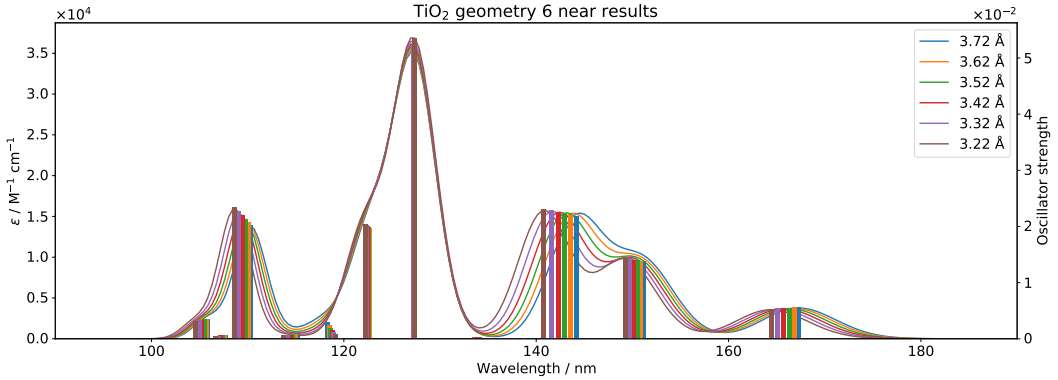


(d) UV-VIS: Formaldehyde in geometry 5. The six nearest distances

Figure 3: Results for TiO_2 geometry 4 and 5



(a) UV-VIS: Formaldehyde in geometry 6. Nearest and farthest distance

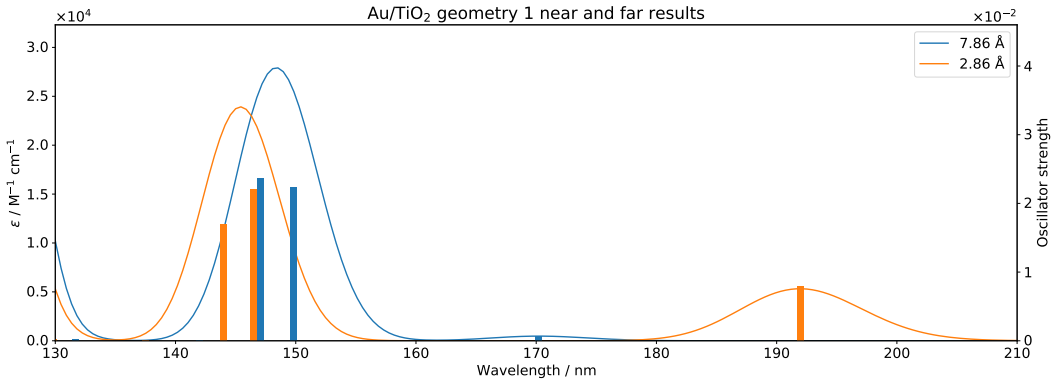


(b) UV-VIS: Formaldehyde in geometry 6. The six nearest distances

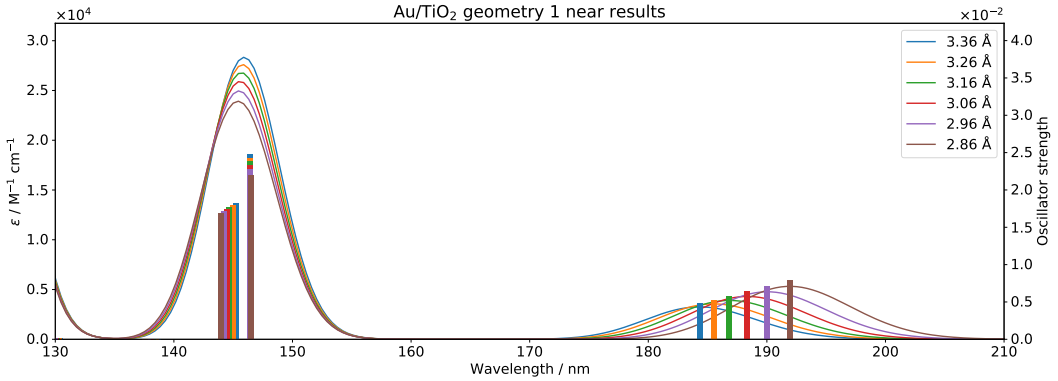
Figure 4: Results for TiO_2 geometry 6

2 UV-Vis spectra for fomaldehyde on Au/TiO_2

Calculated UV-Vis spectra of formaldehyde when placed on the Au/TiO_2-surface. All the excitation energies and oscillator strengths have been calculated with the CCSD linear response method and the aug-cc-pcTZ basis set. For each geometry the difference in the UV-Vis spectra between the closest and farthest position of formaldehyde (near and far results) and the change in the spectra when formaldehyde is in the six closest positions (near results).

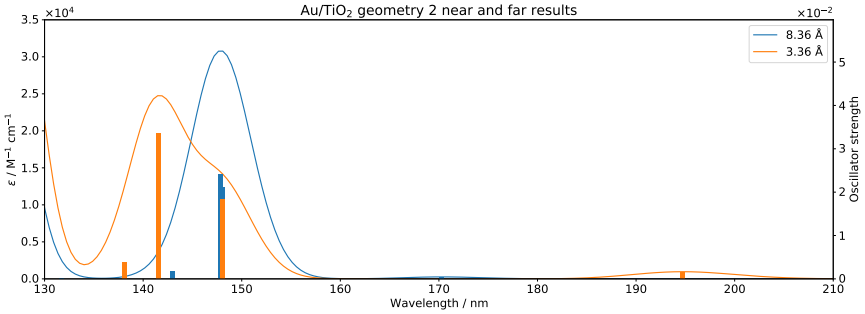


(a) UV-VIS: Formaldehyde in geometry 1. Nearest and farthest distance

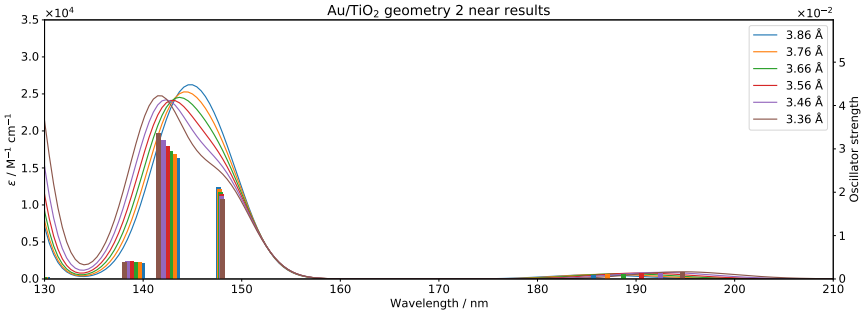


(b) UV-VIS: Formaldehyde in geometry 1. The six nearest distances

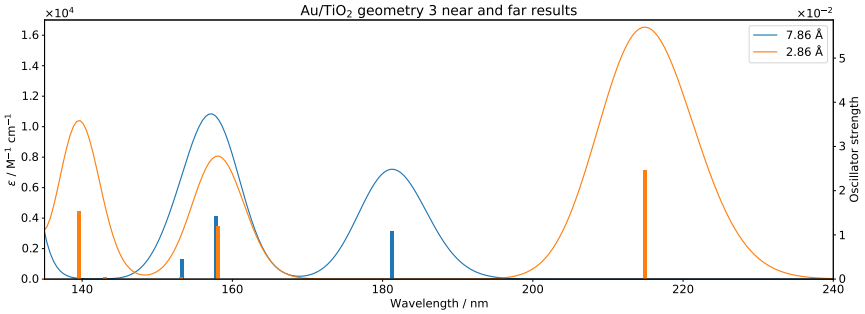
Figure 5: Results for Au/TiO_2 geometry 1



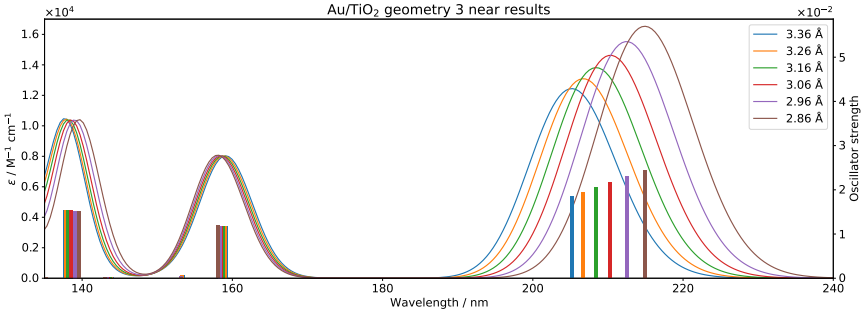
(a) UV-VIS: Formaldehyde in geometry 2. Nearest and farthest distance



(b) UV-VIS: Formaldehyde in geometry 2. The six nearest distances

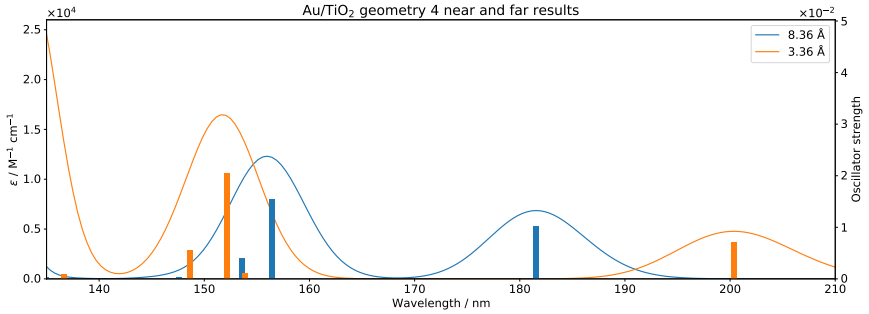


(c) UV-VIS: Formaldehyde in geometry 3. Nearest and farthest distance

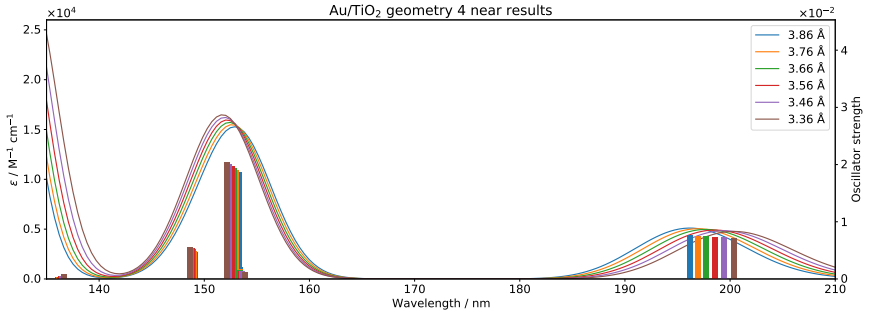


(d) UV-VIS: Formaldehyde in geometry 3. The six nearest distances

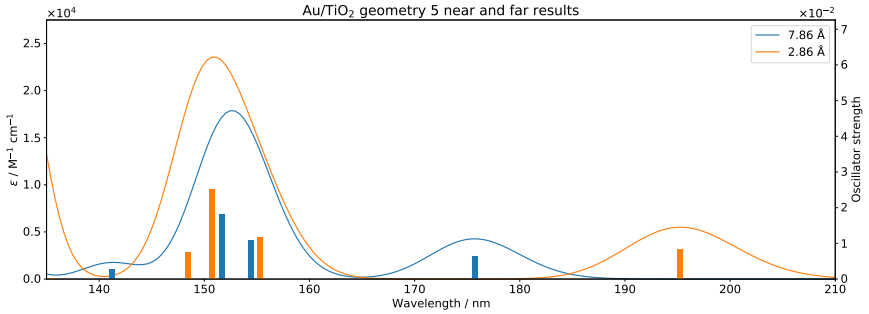
Figure 6: Results for Au/TiO_2 geometry 2 and 3



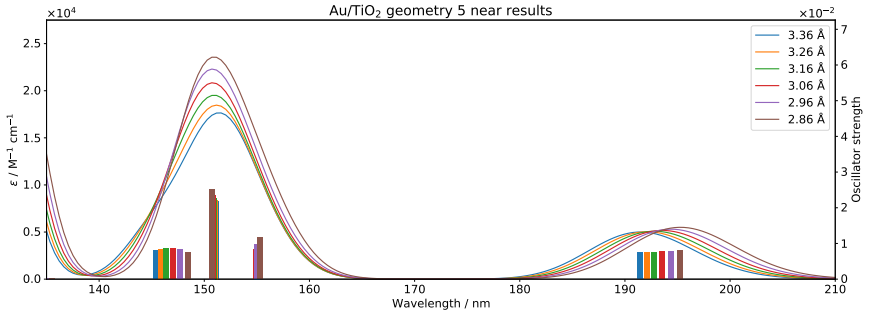
(a) UV-VIS: Formaldehyde in geometry 4. Nearest and farthest distance



(b) UV-VIS: Formaldehyde in geometry 4. The six nearest distances

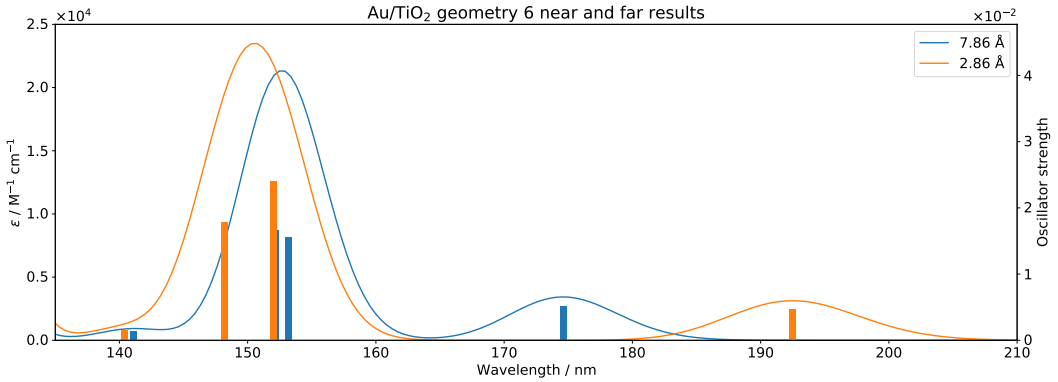


(c) UV-VIS: Formaldehyde in geometry 5. Nearest and farthest distance

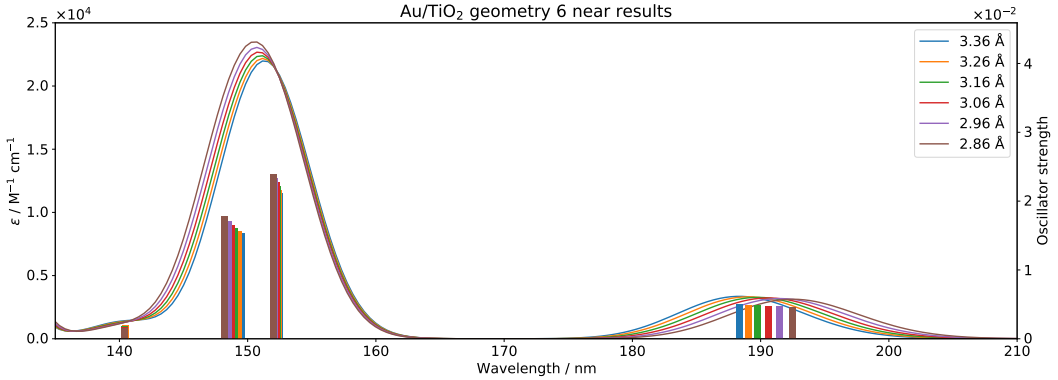


(d) UV-VIS: Formaldehyde in geometry 5. The six nearest distances

Figure 7: Results for Au/TiO_2 geometry 4 and 5



(a) UV-VIS: Formaldehyde in geometry 6. Nearest and farthest distance

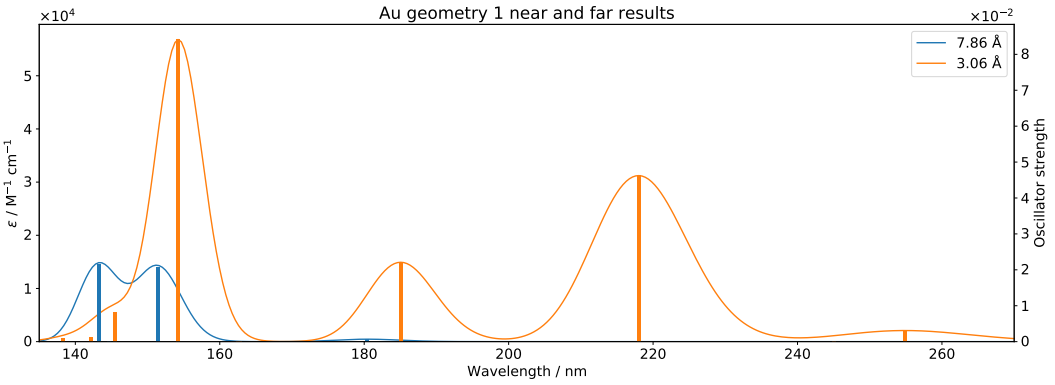


(b) UV-VIS: Formaldehyde in geometry 6. The six nearest distances

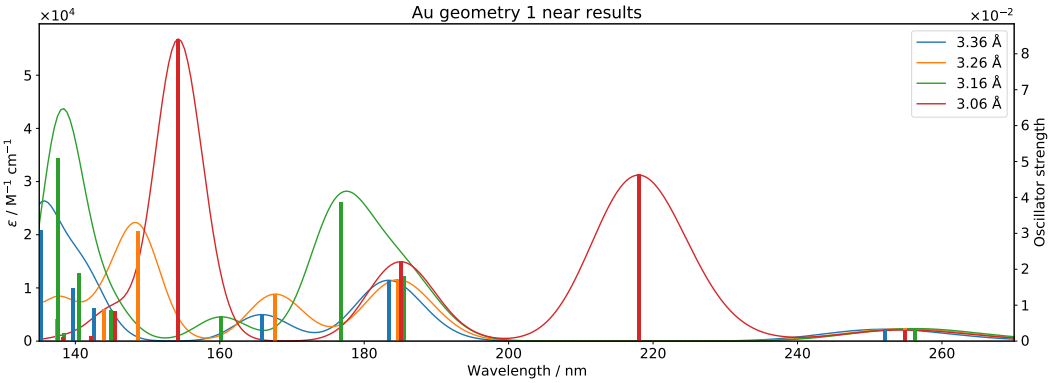
Figure 8: Results for Au/TiO_2 geometry 6

3 UV-Vis spectra for formaldehyde on Au

Calculated UV-Vis spectra of formaldehyde when placed on the gold nanoparticle. All the excitation energies and oscillator strengths have been calculated with the CCSD linear response method and the aug-cc-pcTZ basis set. For each geometry the difference in the UV-Vis spectra between the closest and farthest position of formaldehyde (near and far results) and the change in the spectra when formaldehyde is in the six closest positions (near results).

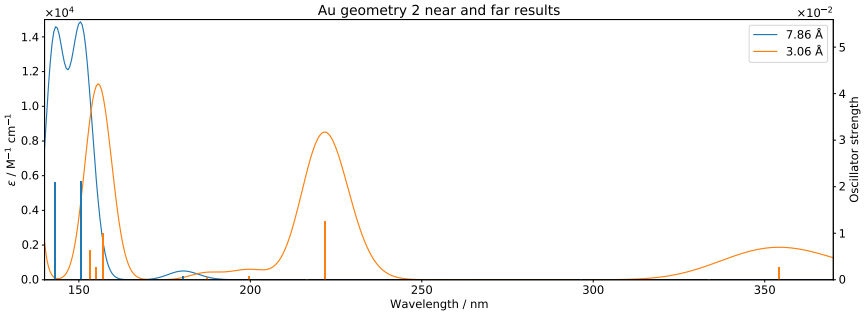


(a) UV-VIS: Formaldehyde in geometry 1. Nearest and farthest distance

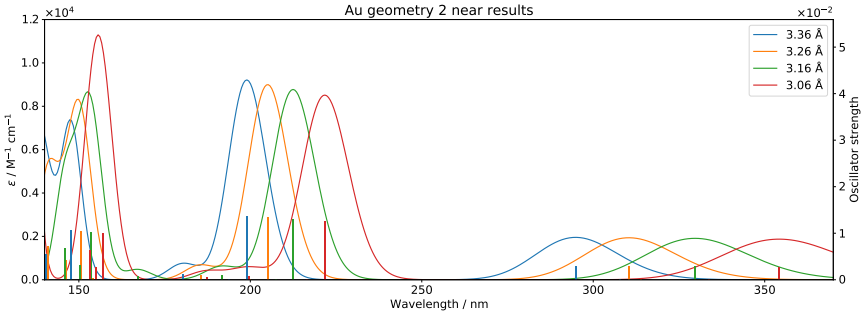


(b) UV-VIS: Formaldehyde in geometry 1. The six nearest distances

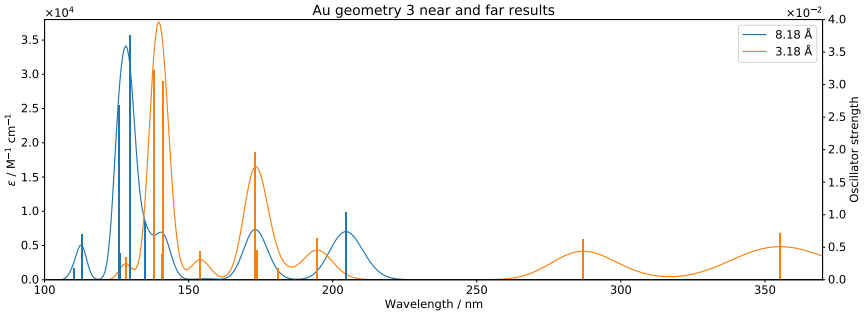
Figure 9: Results for Au geometry 1



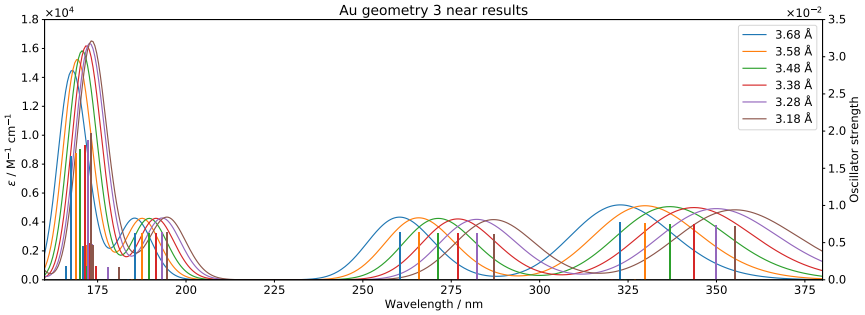
(a) UV-VIS: Formaldehyde in geometry 2. Nearest and farthest distance



(b) UV-VIS: Formaldehyde in geometry 2. The six nearest distances

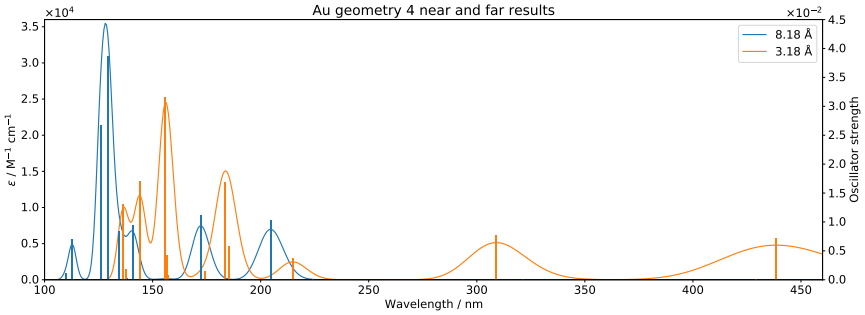


(c) UV-VIS: Formaldehyde in geometry 3. Nearest and farthest distance

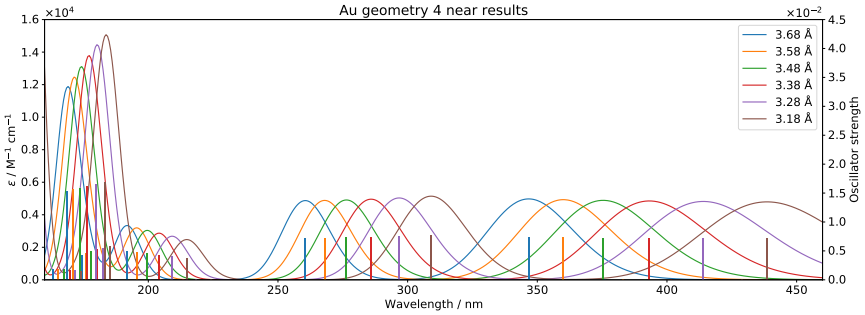


(d) UV-VIS: Formaldehyde in geometry 3. The six nearest distances

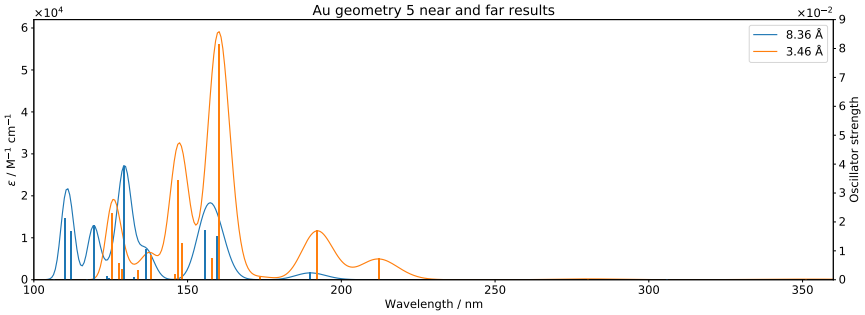
Figure 10: Results for Au geometry 2 and 3



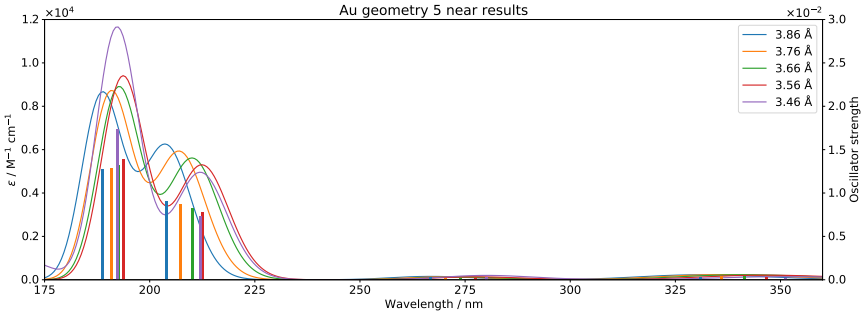
(a) UV-VIS: Formaldehyde in geometry 4. Nearest and farthest distance



(b) UV-VIS: Formaldehyde in geometry 4. The six nearest distances

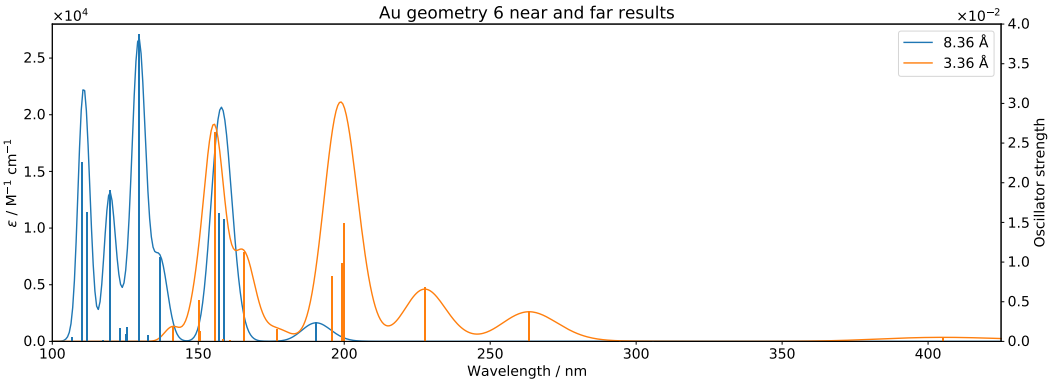


(c) UV-VIS: Formaldehyde in geometry 5. Nearest and farthest distance

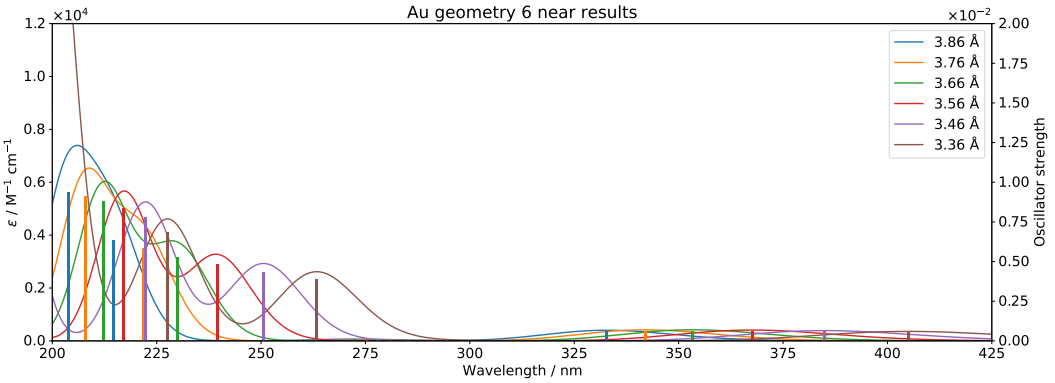


(d) UV-VIS: Formaldehyde in geometry 5. The six nearest distances

Figure 11: Results for Au geometry 4 and 5



(a) UV-VIS: Formaldehyde in geometry 6. Nearest and farthest distance



(b) UV-VIS: Formaldehyde in geometry 1. The six nearest distances

Figure 12: Results for Au geometry 6