Electronic Supporting Information

Systematic theoretical investigation of geometries, stabilities and magnetic properties of iron oxide clusters $(FeO)_n^{\mu}$ (n = 1-8, μ = 0, ±1): Insights and perspectives

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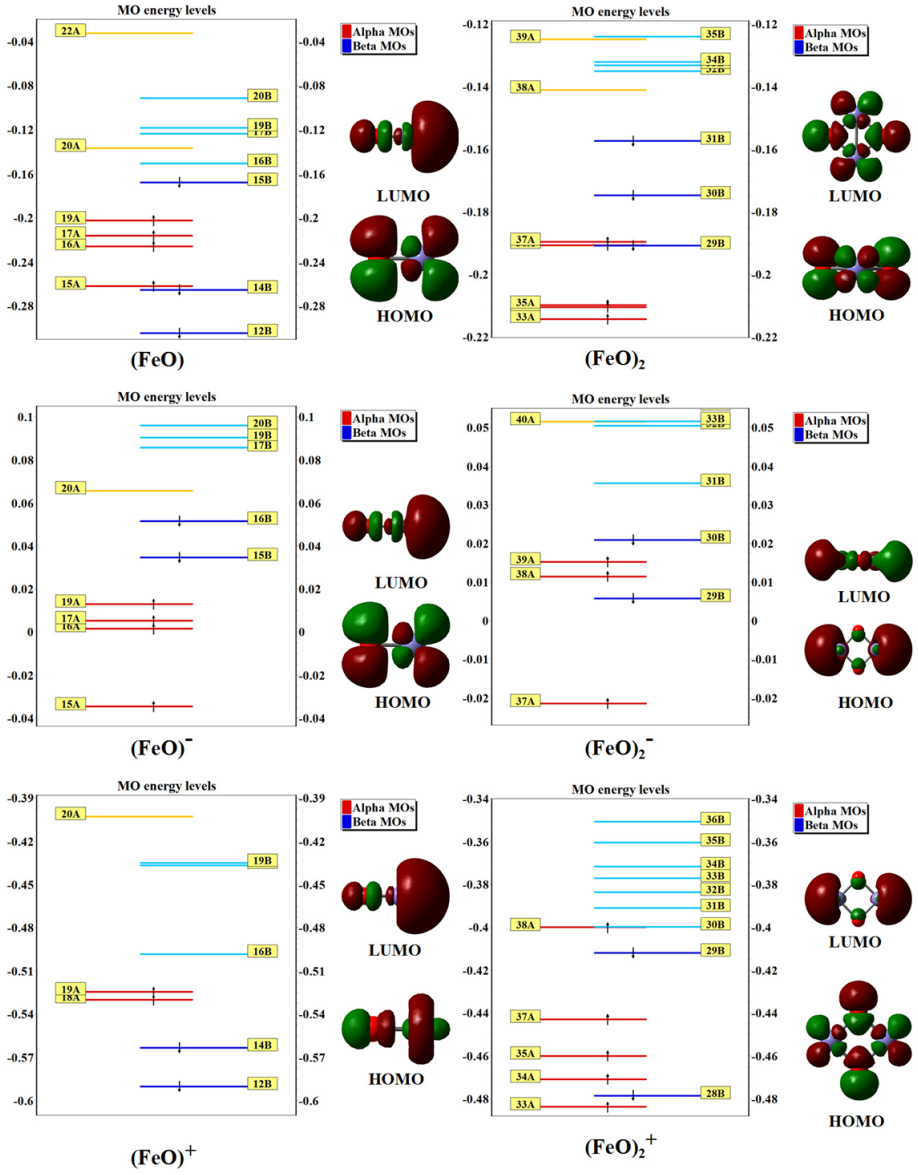

Fig. S1. Calculated molecular orbital energy levels of $(FeO)_n^{\mu}$ (n = 1-2, μ = 0, ±1) clusters together with the molecular orbital maps of the HOMOs and LUMOs.

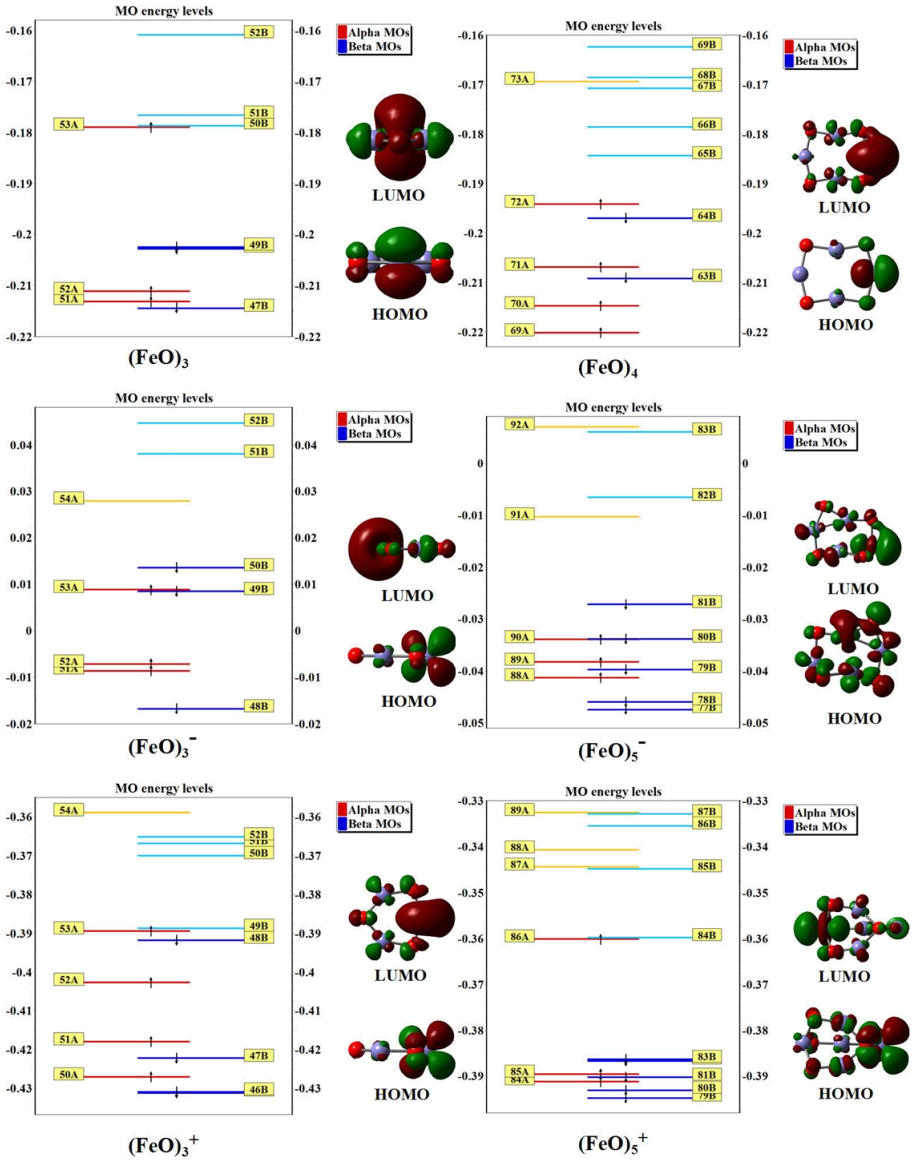

Fig. S2. Calculated molecular orbital energy levels of $(FeO)_n^{\mu}$ (n = 3-5, μ = 0, ±1) clusters together with the molecular orbital maps of the HOMOs and LUMOs.

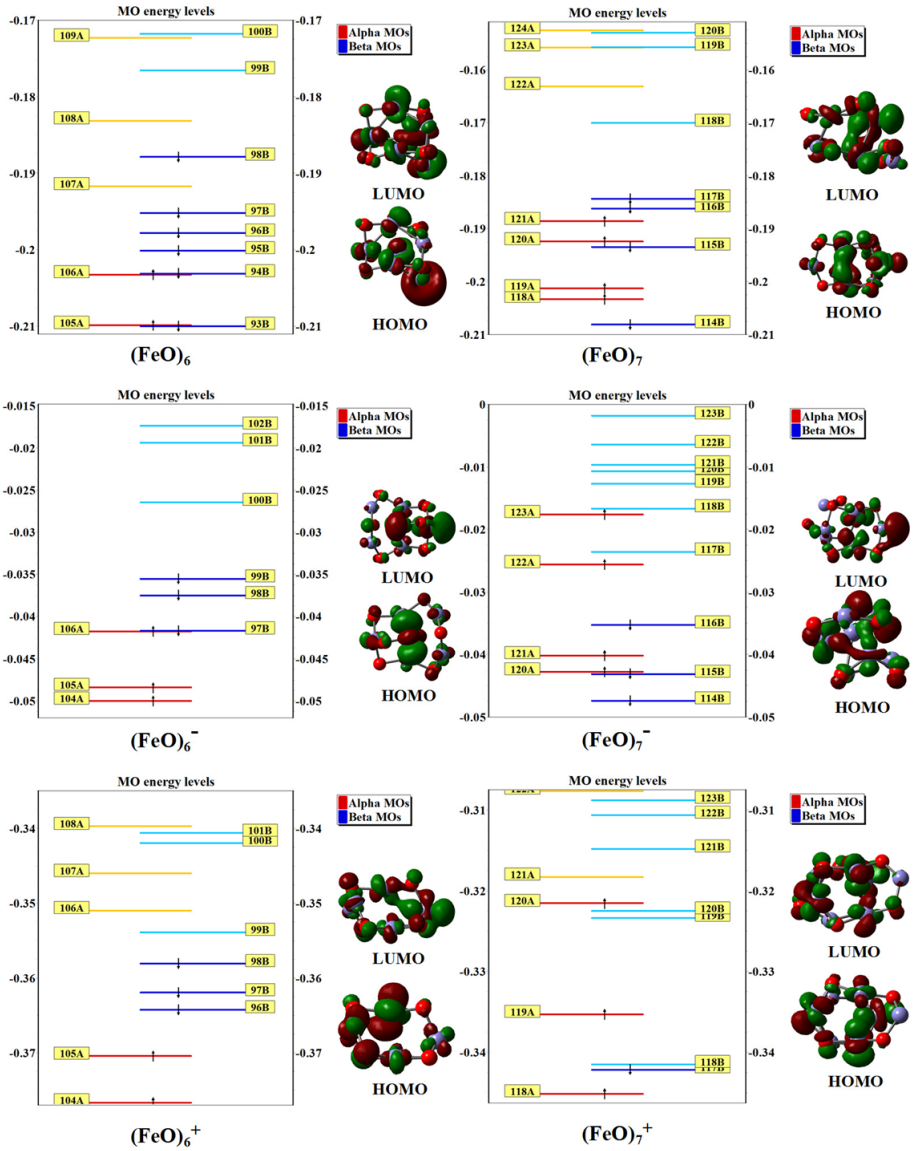

Fig. S3. Calculated molecular orbital energy levels of $(FeO)_n^{\mu}$ (n = 6-7, μ = 0, ±1) clusters together with the molecular orbital maps of the HOMOs and LUMOs.

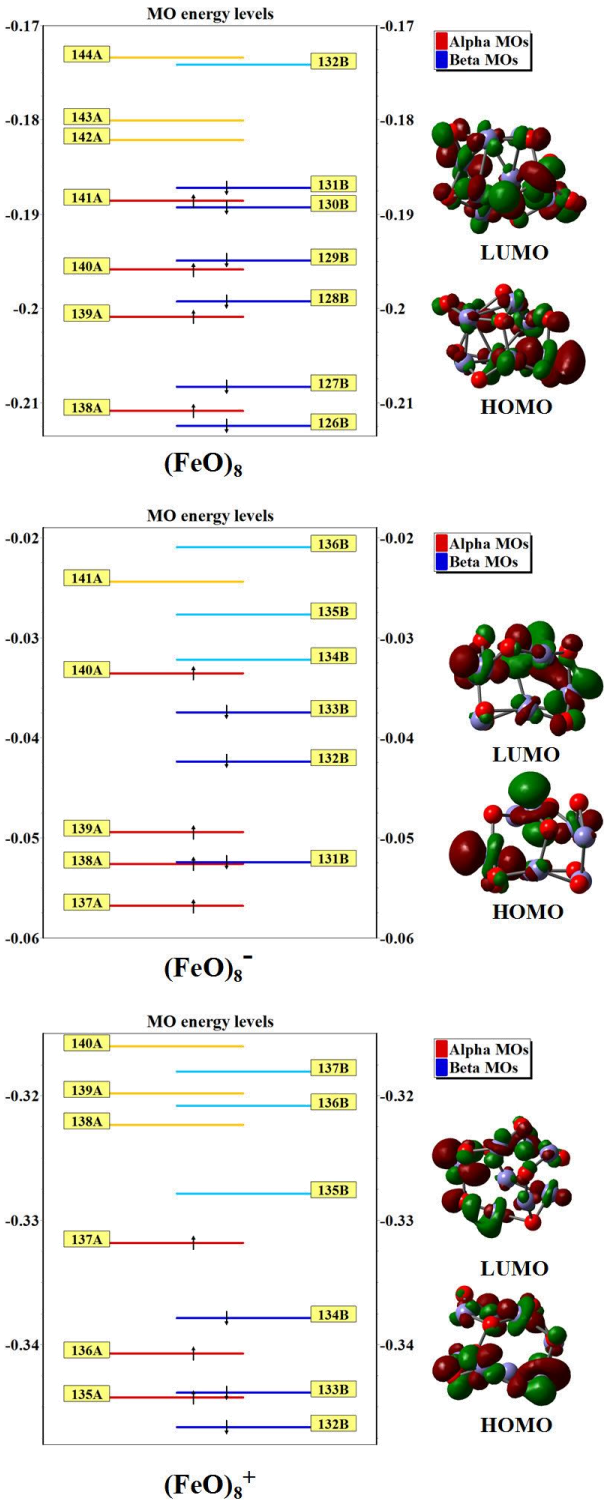

Fig. S4. Calculated molecular orbital energy levels of $(FeO)_n^{\mu}$ (n = 8, μ = 0, ±1) clusters together with the molecular orbital maps of the HOMOs and LUMOs.

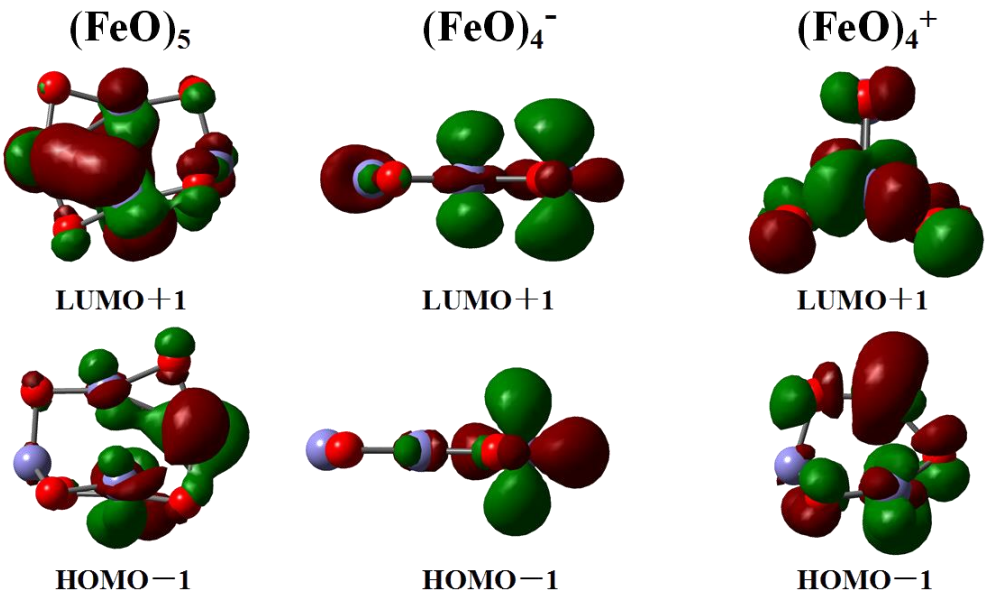

Fig. S5. Calculated molecular orbital maps of the HOMO–1 and LUMO+1 of $(FeO)_5$ and $(FeO)_4^-$ clusters.

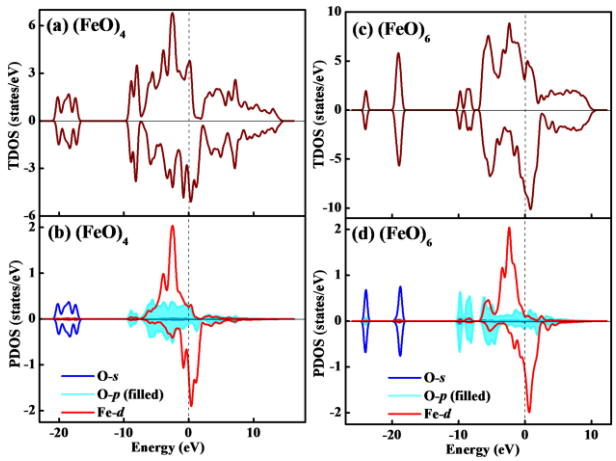

Fig. S6. The calculated total DOS and partial DOS of $(FeO)_4$ and $(FeO)_6$ clusters. The Fermi level is indicated by the vertical dashed line.

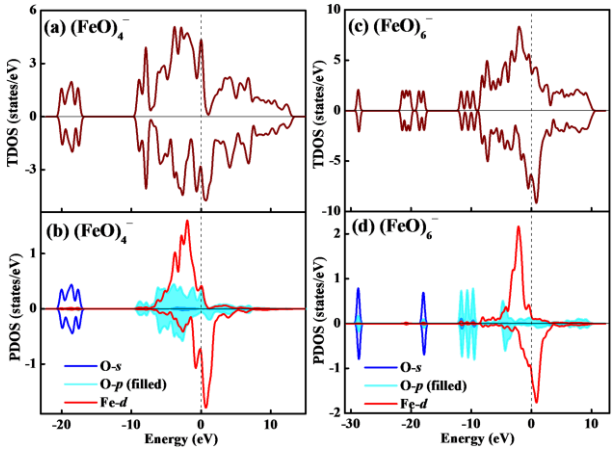

Fig. S7. The calculated total DOS and partial DOS of $(FeO)_4^-$ and $(FeO)_6^-$ clusters. The Fermi level is indicated by the vertical dashed line.

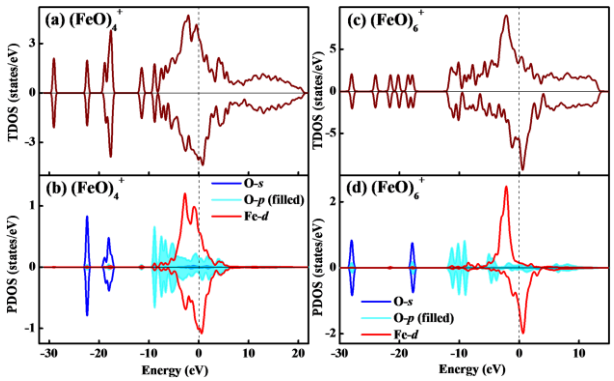

Fig. S8. The calculated total DOS and partial DOS of $(FeO)_4^+$ and $(FeO)_6^+$ clusters. The Fermi level is indicated by the vertical dashed line.

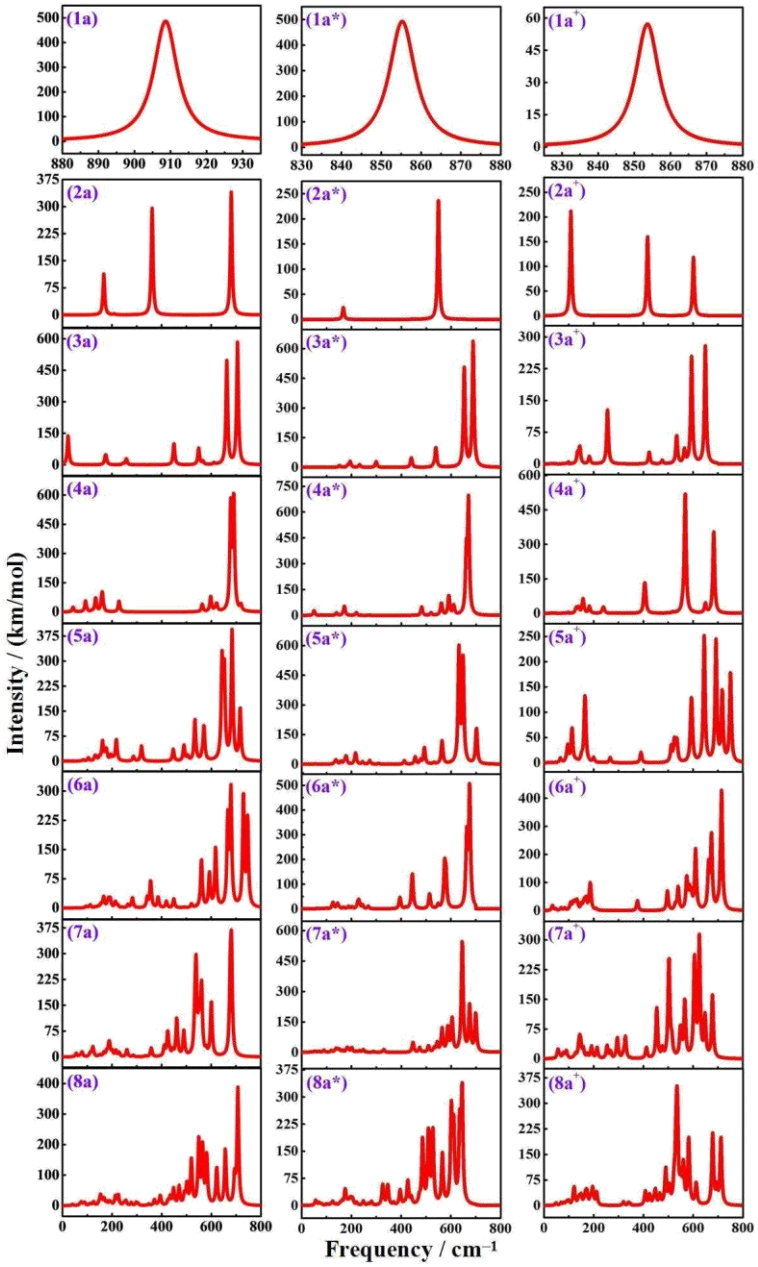

Fig. S9. The calculated infrared spectra of $(FeO)_n^{\mu}$ (n = 1-8, μ = 0, ±1) clusters.

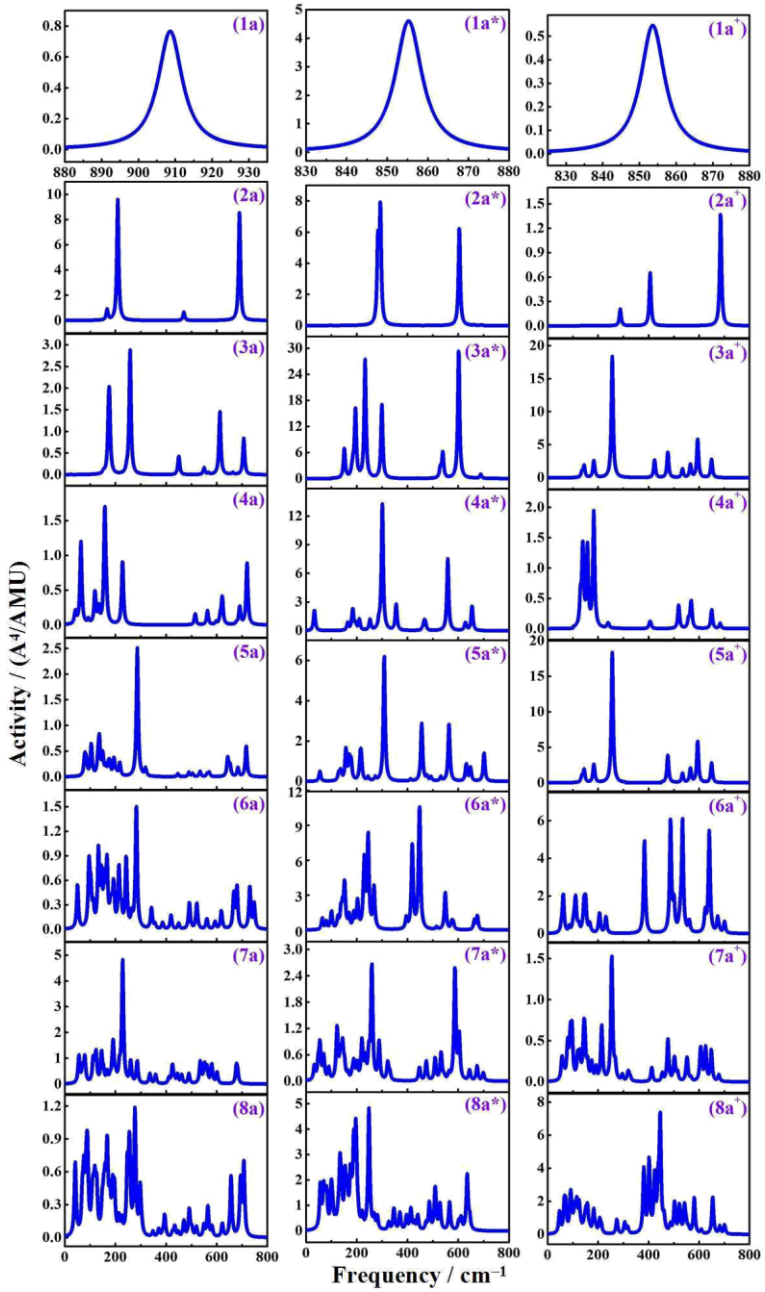

Fig. S10. The calculated Raman spectra of $(FeO)_n^{\mu}$ (n = 1-8, μ = 0, ±1) clusters.

Coordinates of minima. Optimized lowest-energy geometries of neutral, anionic and cationic $(FeO)_n^{\mu}$ (n = 1-8, μ = 0, ±1) clusters at the PW91/6-311+G* level.

1. Neutral clusters

1a FeO

Fe	**0.00000000**	**0.00000000**	**0.37816900**
O	**0.00000000**	**0.00000000**	**-1.22904900**

2a $(FeO)_2$

Fe	**-0.87879000**	**0.71447700**	**-0.00913500**
Fe	**0.87879000**	**-0.71447700**	**-0.00913500**
O	**-0.87879000**	**-1.07811100**	**0.02969000**
O	**0.87879000**	**1.07811100**	**0.02969000**

3a $(FeO)_3$

Fe	**0.00000000**	**0.00000000**	**1.52850400**
Fe	**0.00000000**	**1.17557900**	**-0.73636100**
Fe	**0.00000000**	**-1.17557900**	**-0.73636100**
O	**0.00000000**	**0.00000000**	**-2.12581700**
O	**0.00000000**	**1.70248000**	**0.97226100**
O	**0.00000000**	**-1.70248000**	**0.97226100**

4a $(FeO)_4$

Fe	**0.00000000**	**0.00000000**	**2.18394100**
Fe	**0.00000000**	**1.43313600**	**-0.00983500**
Fe	**0.00000000**	**0.00000000**	**-2.13759600**
Fe	**0.00000000**	**-1.43313600**	**-0.00983500**
O	**0.19125100**	**-1.68365200**	**1.73007400**
O	**0.23477900**	**1.73485600**	**-1.77342200**
O	**-0.19125100**	**1.68365200**	**1.73007400**
O	**-0.23477900**	**-1.73485600**	**-1.77342200**

5a $(FeO)_5$

Fe	**-2.03652300**	**0.21790900**	**-0.10505200**
Fe	**0.00514300**	**-0.67853900**	**1.28476500**
Fe	**2.15125800**	**0.00078600**	**-0.08086200**
Fe	**0.22764200**	**1.51383700**	**-0.03334000**
Fe	**0.05118900**	**-1.27009900**	**-0.99370600**
O	**-1.56156000**	**-0.85709900**	**-1.51548200**
O	**-1.45763500**	**1.90802000**	**-0.32892900**
O	**-1.70699900**	**-0.43425000**	**1.57202500**
O	**2.03511200**	**1.75265700**	**-0.27885800**
O	**1.39527800**	**-1.66698200**	**0.31788000**

6a $(FeO)_6$

Fe	**-2.05078100**	**-0.74949500**	**0.35108300**
Fe	**-1.24612100**	**1.30033400**	**-0.58751800**

Fe	**1.16231400**	**1.45376000**	**-0.41981400**
Fe	**1.83979300**	**-0.85692400**	**-0.03718400**
Fe	**-0.32662000**	**-0.90864800**	**-1.27389500**
Fe	**0.08861900**	**0.17499600**	**1.59090300**
O	**-2.06116900**	**-0.16805900**	**-1.47969200**
O	**1.68096900**	**-0.78755400**	**1.66136300**
O	**1.03876000**	**-2.04266400**	**-0.95930000**
O	**-1.40309500**	**-0.77965300**	**1.97010900**
O	**-0.17291600**	**1.96671000**	**0.78151500**
O	**2.64904000**	**0.46564600**	**-0.75061000**
7a $(FeO)_7$			
Fe	**1.53676700**	**0.77731600**	**1.22322700**
Fe	**1.88384700**	**-1.28071600**	**-0.01112800**
Fe	**-0.87602800**	**1.44707700**	**-0.00765200**
Fe	**-0.63484200**	**-1.11436400**	**-1.13458000**
Fe	**1.45251200**	**1.01813500**	**-1.15061700**
Fe	**-0.65822200**	**-0.77730200**	**1.23921100**
Fe	**-2.92168000**	**-0.06627900**	**0.15955500**
O	**0.74781200**	**2.22714800**	**0.31129200**
O	**0.81693800**	**-2.14892100**	**-1.15697600**
O	**-0.18430900**	**0.54978400**	**-1.86435700**
O	**1.05042700**	**-0.96691300**	**1.79610300**
O	**2.93716600**	**0.32035100**	**-0.13714500**
O	**-2.01176500**	**-1.62723800**	**0.19628400**
O	**-2.64892200**	**1.63322400**	**-0.17875300**
8a $(FeO)_8$			
Fe	**-1.18971400**	**1.09287000**	**1.36688800**
Fe	**0.16136800**	**-0.29519800**	**-1.85760300**
Fe	**0.71656100**	**-1.97923500**	**-0.28285600**
Fe	**-0.21163700**	**-1.10553200**	**1.71626000**
Fe	**-1.75222900**	**-1.02538300**	**-0.07828100**
Fe	**-1.51816000**	**1.22430900**	**-1.01810300**
Fe	**1.11349900**	**2.03095500**	**-0.00699100**
Fe	**2.43167500**	**-0.20067800**	**0.30515900**
O	**2.86131300**	**1.54606800**	**0.29355400**
O	**1.91530900**	**-0.91469600**	**-1.34395100**
O	**-0.77408300**	**-1.93431300**	**-1.42645000**
O	**-2.92800500**	**0.21191600**	**-0.87719400**
O	**0.20866100**	**1.61466100**	**-1.62345300**
O	**-0.02697200**	**2.37817200**	**1.35020100**
O	**1.55017400**	**-1.48748000**	**1.40623000**
O	**-1.99833100**	**-0.57617900**	**1.75152400**

2. Anionic clusters

1a* $(FeO)^-$

Fe	**0.00000000**	**0.00000000**	**0.38346100**
O	**0.00000000**	**0.00000000**	**-1.24625000**

2a* $(FeO)_2^-$

Fe	**-0.92725700**	**0.88185800**	**-0.00030200**
Fe	**0.92725700**	**-0.88185800**	**-0.00030200**
O	**-0.92725700**	**-0.97458000**	**0.00098300**
O	**0.92725700**	**0.97458000**	**0.00098300**

3a* $(FeO)_3^-$

Fe	**0.00000000**	**0.00000000**	**1.50494300**
Fe	**0.00000000**	**1.13103400**	**-0.72533500**
Fe	**0.00000000**	**-1.13103400**	**-0.72533500**
O	**0.00000000**	**0.00000000**	**-2.15318600**
O	**0.00000000**	**1.71973600**	**0.98840200**
O	**0.00000000**	**-1.71973600**	**0.98840200**

4a* $(FeO)_4^-$

Fe	**0.00000000**	**0.00000000**	**2.22966400**
Fe	**0.00010400**	**1.24441700**	**-0.00956300**
Fe	**0.00000000**	**0.00000000**	**-2.18397300**
Fe	**-0.00010400**	**-1.24441700**	**-0.00956300**
O	**0.00099300**	**-1.70197900**	**1.72990300**
O	**0.00000000**	**1.74640900**	**-1.77307100**
O	**-0.00099300**	**1.70197900**	**1.72990300**
O	**0.00000000**	**-1.74640900**	**-1.77307100**

5a* $(FeO)_5^-$

Fe	**0.02974600**	**-2.03220500**	**0.00000000**
Fe	**0.88044200**	**0.13323500**	**1.17139100**
Fe	**-0.25339100**	**2.14197500**	**0.00000000**
Fe	**-1.39439000**	**0.06864800**	**0.00000000**
Fe	**0.88044200**	**0.13323500**	**-1.17139100**
O	**0.88044200**	**-1.58531900**	**-1.58602400**
O	**-1.75101600**	**-1.67392600**	**0.00000000**
O	**0.88044200**	**-1.58531900**	**1.58602400**
O	**-1.99768900**	**1.82471900**	**0.00000000**
O	**1.52355700**	**1.57396200**	**0.00000000**

6a* $(FeO)_6^-$

Fe	**1.97082600**	**-1.19319200**	**-0.01876500**

Fe	**1.77125700**	**1.35265500**	**-0.00842600**
Fe	**-0.61596100**	**1.41836500**	**-0.70334200**
Fe	**-2.27712500**	**-0.11173800**	**0.39068800**
Fe	**0.11787200**	**-0.08993700**	**1.27472400**
Fe	**-0.40092100**	**-1.34368900**	**-0.86753100**
O	**2.07378100**	**0.10640400**	**1.32035200**
O	**-2.14080000**	**-1.58300500**	**-0.66449800**
O	**-1.46482000**	**-0.36773000**	**2.00981600**
O	**1.21384600**	**-2.14459600**	**-1.30238700**
O	**0.85198300**	**2.42570400**	**-1.04096100**
O	**-2.37332400**	**1.45771500**	**-0.54120400**

7a* $(FeO)_7^-$

Fe	**1.32556800**	**0.82943800**	**1.34984700**
Fe	**1.89181800**	**-1.27963700**	**-0.13598300**
Fe	**-0.89338700**	**1.40783000**	**-0.14590000**
Fe	**-0.60547000**	**-0.94307700**	**-1.06488200**
Fe	**1.39827400**	**1.00740700**	**-1.04138700**
Fe	**-0.57279200**	**-0.88094700**	**1.16587100**
Fe	**-2.76242300**	**-0.16137900**	**0.20445500**
O	**0.65481900**	**2.30145300**	**0.43455100**
O	**0.81993600**	**-2.02566500**	**-1.37714000**
O	**-0.18126100**	**0.65557100**	**-1.93654500**
O	**1.15202100**	**-1.01867300**	**1.73826000**
O	**2.90024100**	**0.37173700**	**-0.05288500**
O	**-1.93714600**	**-1.78745100**	**0.25488800**
O	**-2.69877300**	**1.56921800**	**-0.14019300**

8a* $(FeO)_8^-$

Fe	**-0.94195900**	**0.18125500**	**1.55022700**
Fe	**-0.06341000**	**0.39060700**	**-1.62563000**
Fe	**1.41542700**	**-1.43005800**	**-0.85732600**
Fe	**1.02379700**	**-1.38119400**	**1.41135600**
Fe	**-1.11981500**	**-1.84940400**	**-0.13048200**
Fe	**-2.29377400**	**0.48003000**	**-0.50214400**
Fe	**-0.18795100**	**2.26980400**	**0.25929000**
Fe	**2.14041400**	**0.92755400**	**0.01737700**
O	**1.56603400**	**2.62996200**	**0.35264000**
O	**1.84016000**	**0.32238700**	**-1.73540700**
O	**-0.17971600**	**-1.69152100**	**-1.75094900**
O	**-2.80450400**	**-1.20619100**	**-0.44249300**
O	**-1.28759500**	**1.86811000**	**-1.23673000**
O	**-0.87787900**	**1.90789500**	**1.88533400**
O	**2.60448300**	**-0.78559000**	**0.76381300**

O	**-0.77235300**	**-1.70797700**	**1.76511800**

3. Cationic clusters

$1a^{+}$ $(FeO)^{+}$

Fe	**0.00000000**	**0.00000000**	**0.38479300**
O	**0.00000000**	**0.00000000**	**-1.25057800**

$2a^{+}$ $(FeO)_2^{+}$

Fe	**-0.91413100**	**0.89324200**	**-0.00015900**
Fe	**0.91413100**	**-0.89324200**	**-0.00015900**
O	**-0.91413100**	**-0.93524600**	**0.00051800**
O	**0.91413100**	**0.93524600**	**0.00051800**

$3a^{+}$ $(FeO)_3^{+}$

Fe	**-0.01007000**	**1.50978200**	**0.00453400**
Fe	**1.37478400**	**-0.75119600**	**-0.00593200**
Fe	**-1.36460200**	**-0.76859500**	**-0.00677000**
O	**0.01312600**	**-1.93511800**	**0.02731700**
O	**1.65879800**	**0.99456300**	**-0.00150600**
O	**-1.67228900**	**0.97308400**	**0.00073700**

$4a^{+}$ $(FeO)_4^{+}$

Fe	**0.69063400**	**1.36071300**	**0.63446500**
Fe	**0.68918000**	**-1.23047900**	**0.86107300**
Fe	**0.68906500**	**-0.13137300**	**-1.49585000**
Fe	**-1.68290700**	**0.00091300**	**0.00096500**
O	**-1.04522200**	**-0.14688200**	**-1.68123400**
O	**1.87926800**	**-0.00016400**	**-0.00043700**
O	**-1.04348300**	**1.53207300**	**0.71220400**
O	**-1.04497100**	**-1.38429000**	**0.96734900**

$5a^{+}$ $(FeO)_5^{+}$

Fe	**-0.00796200**	**-2.18269500**	**0.00000000**
Fe	**0.90093700**	**0.11205700**	**1.23135500**
Fe	**-0.18230700**	**2.38196400**	**0.00000000**
Fe	**-1.50641500**	**0.06660200**	**0.00000000**
Fe	**0.90093700**	**0.11205700**	**-1.23135500**
O	**0.90093700**	**-1.60448100**	**-1.46733600**
O	**-1.72755000**	**-1.66534400**	**0.00000000**
O	**0.90093700**	**-1.60448100**	**1.46733600**
O	**-1.83145500**	**1.80946900**	**0.00000000**
O	**1.41526100**	**1.47238400**	**0.00000000**

$6a^{+}$ $(FeO)_6^{+}$

Fe	**-1.98905700**	**1.49409800**	**-0.05275200**

Fe	**-1.88410000**	**-1.57661800**	**0.09825500**
Fe	**0.58334700**	**-1.30887700**	**-1.04198600**
Fe	**2.42947900**	**-0.04678000**	**0.52190700**
Fe	**-0.27092100**	**-0.04090500**	**1.29909600**
Fe	**0.59050200**	**1.49073000**	**-0.71383400**
O	**-2.17181700**	**0.01115800**	**1.01987000**
O	**2.27568200**	**1.54211600**	**-0.29916100**
O	**1.31297200**	**-0.28982700**	**1.92671700**
O	**-0.90768800**	**2.32429100**	**-1.12886100**
O	**-1.00233800**	**-2.18977100**	**-1.29044000**
O	**2.25062800**	**-1.43582100**	**-0.58785500**

7a^{+} (FeO)$_{7}^{+}$

Fe	**1.62317900**	**0.89197000**	**1.22597600**
Fe	**1.93118700**	**-1.30059500**	**0.14672700**
Fe	**-0.86296100**	**1.52546900**	**-0.32700700**
Fe	**-0.59194900**	**-1.32622100**	**-1.19554200**
Fe	**1.55064500**	**0.94299800**	**-1.16522100**
Fe	**-0.73210500**	**-0.68382800**	**1.24432400**
Fe	**-3.14878300**	**-0.02976700**	**0.27452300**
O	**0.74572100**	**2.20240300**	**0.20544700**
O	**0.86144700**	**-2.28932900**	**-0.87891600**
O	**-0.13228800**	**0.40725500**	**-1.82344000**
O	**0.95638000**	**-0.78616200**	**1.83227900**
O	**2.97823700**	**0.27721000**	**-0.07876300**
O	**-2.03519400**	**-1.46916400**	**0.16048300**
O	**-2.62424300**	**1.59270400**	**-0.07937800**

8a^{+} (FeO)$_{8}^{+}$

Fe	**-1.62806700**	**0.32406600**	**1.40976700**
Fe	**0.28457700**	**-0.24500500**	**-1.67039700**
Fe	**2.07976000**	**-1.33275600**	**-0.29029200**
Fe	**0.59774600**	**-0.79506100**	**1.77625800**
Fe	**-0.97179400**	**-1.99330900**	**-0.03097900**
Fe	**-2.11959800**	**0.14842400**	**-1.01035900**
Fe	**-0.47537900**	**2.49026200**	**-0.13219900**
Fe	**2.15724300**	**1.16261000**	**0.13982500**
O	**1.25598600**	**2.64740500**	**0.22239000**
O	**2.10108900**	**0.24863300**	**-1.46284900**
O	**0.56993500**	**-2.10233200**	**-1.19122200**
O	**-2.49653700**	**-1.53904800**	**-0.89055500**
O	**-0.81799400**	**1.31313600**	**-1.63429400**
O	**-1.58067000**	**2.03927300**	**1.21624600**
O	**2.31926700**	**-0.37780000**	**1.33016300**

O	**-1.10566000**	**-1.44677000**	**1.78734600**