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Electronic Supplementary Information: Support effects on conical intersections of Jahn-Teller fluxional metal clusters on the sub-nanoscale.

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Table 1 Cartesian coordinates of Cu_3–benzene complex optimized at CCSD(T) level of theory with the (A)VTZ-PP basis set (see Methods section of the main manuscript).

Cu	0.0000000000	0.0000000000	2.1647011780
Cu	1.1965698226	0.0000000000	0.1452150968
Cu	−1.1965698226	0.0000000000	0.1452150968
C	1.4393562644	0.0000000000	−1.8668074845
C	0.6891623209	1.2327787744	−2.0438192718
C	−0.6891623209	1.2327787744	−2.0438192718
C	−1.4393562644	0.0000000000	−1.8668074845
C	−0.6891623209	−1.2327787744	−2.0438192718
C	0.6891623209	−1.2327787744	−2.0438192718
H	2.4930222766	0.0000000000	−2.1266921421
H	1.2275673417	2.1667866008	−2.1551182346
H	−1.2275673417	2.1667866008	−2.1551182346
H	−2.4930222766	0.0000000000	−2.1266921421
H	−1.2275673417	−2.1667866008	−2.1551182346
H	1.2275673417	−2.1667866008	−2.1551182346

Table 2 Cartesian coordinates of benzene optimized at CCSD(T) level of theory with the VTZ-PP basis set (see Methods section of the main manuscript).

C	0.0000000000	1.3975343043	0.0000107037
C	−1.2103050738	0.6987689685	−0.0000037014
C	−1.2103050738	−0.6987689685	−0.0000037014
C	0.0000000000	−1.3975343043	0.0000107037
C	1.2103050738	−0.6987689685	−0.0000037014
C	1.2103050738	0.6987689685	−0.0000037014
H	0.0000000000	2.4806619448	−0.0000269835
H	−2.1483156187	1.2403389412	−0.0000061758
H	−2.1483156187	−1.2403389412	−0.0000061758
H	0.0000000000	−2.4806619448	−0.0000269835
H	2.1483156187	−1.2403389412	−0.0000061758
H	2.1483156187	1.2403389412	−0.0000061758

Python code delivering a two-dimensional representation of relaxed potential energy surface scans of Cu_3–benzene in two crossing electronic states is available in the plot.txt (plot.py) file. Data containing θ angles (in degrees), Z distances (in Å) and relative energies (in eV) for both states are available in the data.txt and theta60.txt files.

Table 3 Numerical values of Cu_3−benzene uncoupled dispersion (E_{disp}^{UHF}), coupled dispersion ($E_{disp}^{TD\text{-}UHF}$) contributions, difference between them (ΔE_{disp}^{UHF}) (in cm^{-1}) and values of the square of the coefficient of the main configuration in the reference wavefunction (CI^2) for the orthogonal and parallel configurations.

	E_{disp}^{UHF}	$E_{disp}^{TD\text{-}UHF}$	ΔE_{disp}	CI^2
orthogonal	−27269	−23842	3427	0.8822
parallel	−8503	−7174	1329	0.8977

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