

Supplementary Information for Reduction of the Molecular Hamiltonian Matrix using Quantum Community Detection

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Supplementary Results

Expanded tables are shown with more details including molecule point groups, FCI energies, and cluster energies. Additional *k*-clustering results are also included.

Molecules using FCI and the sto-3g minimal basis set. Molecules created using FCI and the sto-3g minimal basis set are shown in Table S 1. Table S 2 shows the energy for the H₂O ground state and next five excited states for the reduced matrices based on the communities of size 65 (CL65) and 52 (CL52). Chemically accurate energies for five excited states are shown for CL65 and only the first three for CL52.

Molecules using the CASSCF method. Table S 4 shows extended data for molecules using the CASSCF method in addition to what is shown in the main manuscript. The choice of active space for the benzene, caffeine, and ferrocene molecules is shown in Figure S 1.

Molecules using other truncation methods and extended basis sets. Table S 3 shows molecules with different truncation methods and extended basis sets. Results with energy differences within chemical accuracy are highlighted. Molecule matrices of SDs created using the CIS truncation (CI + single excitations) are chemically known to have the first determinant in the matrix (the Hartree-Fock determinant) result as the lowest eigenvalue. This means there is no correlation between the first SD and any of the other SDs. This community of 1 SD is discovered at $k = 5$ for the 2 benzene examples in Table S 3. The energy difference remains the same for $k = 2$ to $k = 5$ since this 1 SD is present in all.

Table S 1: Molecules using the FCI method and the sto-3g minimal basis set.

Molecule (Point Group)	Size	E_{FCI} (Hartree)	E_{CL} (Hartree)	k	Reduced Size	$E_{CL} - E_{FCI}$ (kcal/mol)
H ₂ O (C _{2v})	133	-75.02039100	-75.02031690	2	65	0.05
			-75.01930565	4	52	0.68
CO (C _{∞v} ⇒ C _{2v})	3648	-111.36801449	-111.36799244	2	2013	0.01
			-111.36793125	2	1768	0.05
			-111.36793125	3	1768	0.05
			-111.36016556	4	1143	4.92
			-111.36770868	5	792	0.19
CH ₄ (T _d ⇒ C _{2v})	4076	-39.80512049	-39.80484039	2	2284	0.18
			-39.80469968	3	1284	0.26
BH ₄ ⁻ (T _d ⇒ C _{2v})	4076	-26.61685162	-26.61639066	2	2284	0.29
			-26.61620071	3	1284	0.41
H ₄ O ²⁺ (C ₁)	15876	-75.36527671	-75.36519709	2	8820	0.05
			-75.36514440	3	4900	0.08
BH ₃ (C _{2v})	1250	-26.12145752	-26.11717567	2	625	2.69
			-26.12097251	3	321	0.30
N ₂ (D _{∞h} ⇒ D _{2h})	1824	-107.66863149	-107.66247136	2	1036	3.87
			-107.65620751	3	648	7.80
			-107.66241960	4	544	3.89
			-107.66835021	5	396	0.18
			-107.66835021	6	396	0.18

Table S 2: Excited States for H₂O.

Excited State	E_{FCI} (Hartree)	E_{CL65} (Hartree)	$E_{CL65} - E_{FCI}$ (kcal/mol)	E_{CL52} (Hartree)	$E_{CL52} - E_{FCI}$ (kcal/mol)
0	-75.02039100	-75.02031690	0.05	-75.01930565	0.68
1	-74.53743573	-74.53734050	0.06	-74.53713325	0.19
2	-74.43197396	-74.43183640	0.09	-74.43118524	0.49
3	-74.31751274	-74.31748072	0.02	-74.31670398	0.51
4	-74.07950770	-74.07943762	0.04	-74.02668361	33.15
5	-74.00260411	-74.00238742	0.13	-73.97540263	17.07

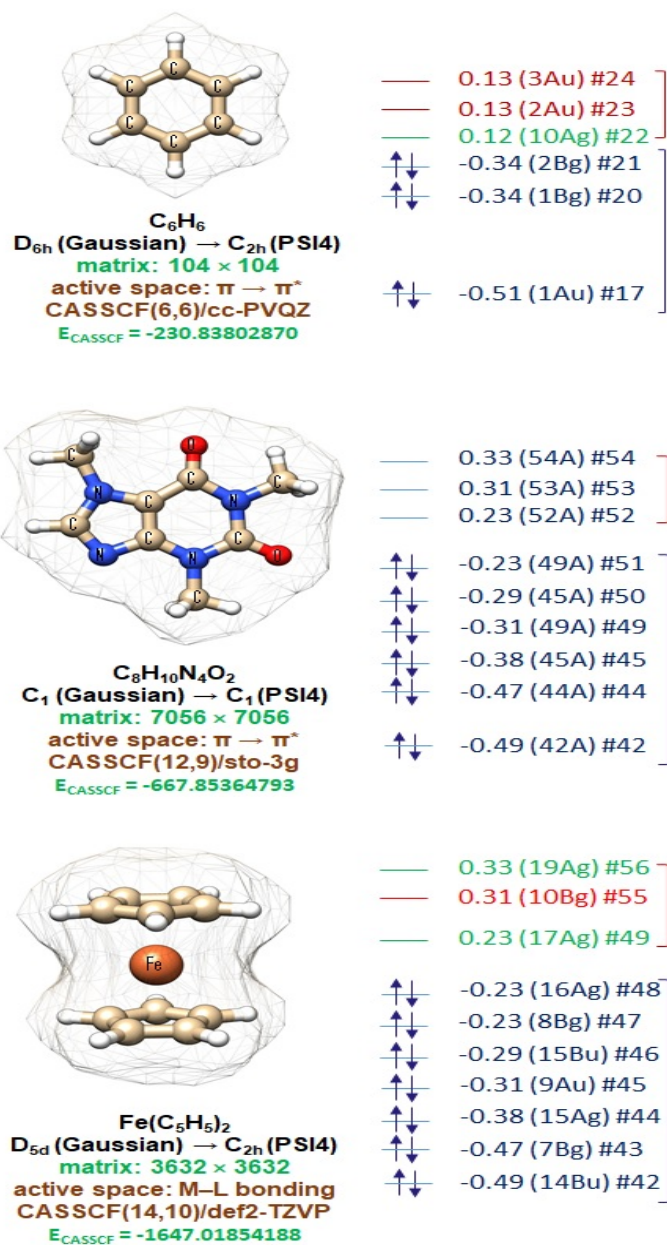


Figure S 1: Chemically-inspired choice of active space for CASSCF calculations of benzene (top), caffeine (middle) and ferrocene (bottom). For each numbered molecular orbital, energy (in Hartree) and irreducible representation is shown.

Table S 3: Molecules using CIS and extended basis sets.

Molecule (Point Group)	Basis Set	Size	E_{CL} (Hartree)	k	Reduced Size	$E_{CL} - E_{FCI}$ (kcal/mol)
C ₆ H ₆ Benzene (D _{6h})	6-31G*	591	-230.70313698	2	191	4.99e-10
				3	115	4.99e-10
				4	96	4.99e-10
				5	1	4.99e-10
C ₆ H ₆ Benzene (D _{6h})	cc-PVDZ	651	-230.72234960	2	207	5.35e-10
				3	104	5.35e-10
				5	1	5.35e-10

Comparison with other methods. In addition to the figure in the main manuscript, Table S 5 and Table S 6 show *Quantum Community Detection* (QCD) compared to other methods, currently in practice, CISD, CISDT, CCSD(T), CISDTQ, and FCI for 5 molecules. Size and energy are shown for N₂, CO, H₄O²⁺, BH³, and H₂O. QCD is comparable in energy and size for these 5 molecules.

N₂ bond dissociation. A bond dissociation energy experiment was performed for N₂ for distances of 0.5 to 2.4 Å. The ground state for each N₂ matrix was optimized using the restricted Hartree-Fock (RHF) method and the sto-3g basis set. The Hamiltonian matrices were generated using Psi4¹ along with the rHF and rFCI energies. Low energy communities were discovered for each bond distance using our *Quantum Community Detection* approach producing energies well within chemical accuracy as seen in the figures in the main manuscript and Table S 7. Interestingly, the $E_{fCL} - E_{rFCI}$ values decrease with increasing bond distance. The reduced sub-matrices are all similar in size ranging from 363 to 397 SDs (see Table S 7) as compared to the original 1824 SDs, up to a 25% reduction in size.

H₃O⁺ bond dissociation. The Tables S 8, S 9, and S 10 show all results from all *k*-clusterings that appear in the figures in the main text and more. A bond dissociation energy experiment was performed for H₃O⁺ for O-H bond distances of 0.39 to 3.39 Å. We simulated a constrained potential energy surface of an oxonium ion (or hydronium cation) (H₃O⁺) in sto-3g basis (FCI method). Specifically, the constrained parameter was chosen as an O-H bond. Starting from the optimized geometry of H₃O⁺, the latter was stretched/shortened by using a step of 0.2 Å in a constrained scan optimization (HF). The overall process can be viewed as a protonation of H₂O. The optimized geometries were used to generate FCI matrices of size 3136. The *Quantum Community Detection* method produced reduced matrices of size 1576 for all geometries, a 50% reduction.

Table S 4: Molecules using the CASSCF method.

Molecule (Point Group)	Basis Set	Size	E_{CL} (Hartree)	k	Reduced Size	$E_{CL} - E_{FCI}$ (kcal/mol)
HCN (10,8) Hydrogen Cyanide (C ₁)	sto-3g	1576	-91.82114958	2	792	0.000013
HCN (10,9) Hydrogen Cyanide (C ₁)	sto-3g	8036	-91.84350714	2	4076	0.000054
HCN (10,9) Hydrogen Cyanide (C ₁)	6-31G*	4076	-93.00896883	2	2110	5.15
H ₂ O (8,8) Water (C _s)	cc-PVDZ	1234	-76.10109262	2	617	0.35
(CH ₃) ₂ CO (20,12) Acetone (C _{2v})	def2-svp	2186	-191.89079792	2	1027	0.07
			-191.89090301	3	661	0.0082
			-191.89089957	4	455	0.01
			-191.89089583	5	340	0.01
			-191.89079142	6	391	0.08
			-191.89079142	7	384	0.08
			-191.89089583	8	343	0.01
(CH ₃) ₂ CO (20,12) Acetone (C _{2v})	6-31G*	1098	-191.89079067	9	209	0.08
			-192.03451734	2	513	0.08
			-192.03456810	3	304	0.04
			-192.03451389	4	208	0.08
(CH ₃) ₂ CO (20,12) Acetone (C _{2v})	cc-PVDZ	1098	-192.05021581	2	481	0.04
			-192.05021210	3	303	0.05
			-192.05015569	4	208	0.08
C ₆ H ₆ (6,6) Benzene (D _{6h})	cc-PVQZ	104	-230.83691596	2	52	0.70
			-230.83688457	3	28	0.72
			-230.83688457	4	28	0.72
C ₈ H ₁₀ N ₄ O ₂ (12,9) Caffeine (C ₁)	sto-3g	7056	-667.81482548	2	3920	24.36
			-667.81195537	3	2352	26.16
			-667.81195537	4	2352	26.16
			-667.80878930	5	784	28.15
			-667.80878930	6	784	28.15
Fe(C ₅ H ₅) ₂ (14,10) Ferrocene (D _{5d})	def2-TZVP	3532	1647.01843406	2	1800	0.68
			-1647.01800674	3	1592	0.33
			-1647.01627361	4	1052	1.42

Table S 5: Energy comparison to other methods.

Method	N ₂ energy (kcal/mol)	CO energy (kcal/mol)	H ₄ O ²⁺ energy (kcal/mol)	BH ₃ energy (kcal/mol)	H ₂ O energy (kcal/mol)
CISD	-96.35	-81.18	-47.68	-31.08	-33.64
CISDT	-97.59	-85.42	-48.23	-31.28	-33.70
CCSD(T)	-103.74	-88.91	-49.47	-31.77	-34.16
CISDTQ	-105.19	-88.92	-49.46	-31.84	-34.19
QCD	-105.23	-89.27	-49.49	-31.85	-34.15
FCI	-105.41	-89.46	-49.54	-31.85	-34.19

Table S 6: Size comparison to other methods.

Method	N ₂ size	CO size	H ₄ O ²⁺ size	BH ₃ size	H ₂ O size
CISD	92	162	561	361	49
CISDT	396	790	3041	1545	105
CCSD(T)	396	2173	8251	3355	133
CISDTQ	1083	2173	8251	3355	133
QCD	396	792	8820	2450	65
FCI	1824	3648	15876	4900	133

Table S 7: N₂ Bond Dissociation.

Bond Distance	Size	E_{CL} (Hartree)	k	Reduced Size	Δ_{FCI-CL} (kcal/mol)
0.83385	1824	-106.98489234	2	396	0.23
0.93385	1824	-107.40247938	2	396	0.22
1.03385	1824	-107.59714601	2	396	0.20
1.13385	1824	-107.66835022	2	396	0.18
1.23385	1824	-107.67420956	2	396	0.15
1.33385	1824	-107.64815357	2	397	0.13
1.43385	1824	-107.60908805	2	396	0.11
1.53385	1824	-107.56762396	2	396	0.09
1.63385	1824	-107.52984467	2	396	0.07
1.73385	1824	-107.49914796	2	336	0.06
1.83385	1824	-107.47668893	2	336	0.04
1.93385	1824	-107.46173680	2	396	0.03
2.03385	1824	-107.45250906	2	396	0.02
2.13385	1824	-107.44709122	2	396	0.01
2.23385	1824	-107.44396273	2	396	0.01
2.33385	1824	-107.44211517	2	398	0.008

Table S 8: H₃O⁺ Bond Dissociation.

Bond Distance	Size	E_{CL} (Hartree)	k	Reduced Size	$E_{CL} - E_{FCI}$ (kcal/mol)
0.39	3136	-73.21424520	2	1576	9.99e-10
		-73.21424520	3	846	3.65e-08
		-73.21424520	4	846	3.65e-08
		-73.21413644	5	429	0.07
		-73.21318913	6	625	0.66
0.59	3136	-74.90123035	2	1576	9.45e-10
		-74.90123035	3	846	9.70e-07
		-74.90123035	4	846	9.70e-07
		-74.90108487	5	429	0.09
		-74.90108487	6	429	0.09
0.79	3136	-75.31375455	2	1576	4.99e-10
		-75.31375455	3	846	2.52e-07
		-75.31375455	4	846	2.52e-07
		-75.31361997	5	429	0.08
		-75.31361997	6	429	0.08
0.99	3136	-75.39362382	2	1576	1.57e-05
		-75.39350794	3	1225	0.07
		-75.39350791	4	625	0.07
		-75.39350791	5	625	0.07
		-75.39350791	6	625	0.07
1.19	3136	-75.37484922	2	1576	1.75e-09
		-75.37474839	3	1225	0.06
		-75.37474839	4	625	0.06
		-75.37477659	5	925	0.04
		-75.37474839	6	625	0.06
1.39	3136	-75.32919311	2	1576	5.35e-11
		-75.32916457	3	1276	0.02
		-75.32910307	4	625	0.06
		-75.32910307	5	625	0.06
		-75.32910307	6	625	0.06
1.59	3136	-75.28151591	2	1576	9.01e-10
		-75.28143317	3	1225	0.05
		-75.28146194	4	925	0.03
		-75.28146194	5	925	0.03
		-75.28143317	6	625	0.05

Table S 9: H₃O⁺ Bond Dissociation (cont'd).

Bond Distance	Size	E_{CL} (Hartree)	k	Reduced Size	$E_{CL} - E_{FCI}$ (kcal/mol)
1.79	3136	-75.24069954	2	1576	8.92e-10
		-75.24062156	3	1225	0.05
		-75.24065014	4	925	0.03
		-75.24065014	5	925	0.03
		-75.24062156	6	625	0.05
1.99	3136	-75.21042253	2	1576	5.35e-11
		-75.21034748	3	1225	0.05
		-75.21037542	4	925	0.03
		-75.21037542	5	825	0.03
		-75.21034748	6	625	0.05
2.19	3136	-75.19122570	2	1576	2.32e-10
		-75.19119874	3	1276	0.02
		-75.19117922	4	925	0.03
		-75.19116894	5	890	0.03
		-75.19115215	6	625	0.05
2.39	3136	-75.18083769	2	1576	4.46e-11
		-75.18081149	3	1276	0.02
		-75.18079089	4	925	0.03
		-75.18079089	5	925	0.03
		-75.18076457	6	625	0.04
2.59	3136	75.17583704	2	1576	6.06e-10
		-75.17576383	3	1077	0.04
		-75.17576399	4	781	0.04
		-75.17576383	5	625	0.04
		-75.17576383	6	625	0.04
2.79	3136	-75.17359540	2	1576	1.25e-10
		-75.17359479	3	1220	0.00039
		-75.17352726	4	897	0.04
		-75.17352193	5	625	0.05
		-75.17352193	6	625	0.05
2.99	3136	-75.17262462	2	1576	3.57e-10
		-75.17255090	3	1225	0.05
		-75.17262388	4	1020	0.00046
		-75.17255090	5	625	0.05
		-75.17255090	6	625	0.05

Table S 10: H₃O⁺ Bond Dissociation (cont'd).

Bond Distance	Size	E_{CL} (Hartree)	k	Reduced Size	$E_{CL} - E_{FCI}$ (kcal/mol)
3.19	3136	-75.17220417	2	1576	6.06e-10
		-75.17180634	3	1184	0.25
		-75.17189117	4	864	0.20
		-75.16958650	5	760	1.64
		-75.16947167	6	584	1.71
3.39	3136	75.17202395	2	1576	4.19e-10
		-75.17069160	3	1176	0.84
		-75.17069162	4	792	0.84
		-75.17069162	5	792	0.84
		-75.17069160	6	584	0.84

Derivation for the gauge metric. In order to derive an expression for a metric function that could be used to gauge the energy difference in the main manuscript, let's consider a Hamiltonian matrix H composed of only two interacting states¹. That is, we suppose that if state i and j are interacting through V_{ij} , the result of their interaction will not be affected by a third state. We have, hence, a collection of so called “two-level systems” represented by the following Hamiltonian matrices:

$$\left\{ \begin{bmatrix} \epsilon_{ii} & V_{ij} \\ V_{ij} & \epsilon_{jj} \end{bmatrix} \right\}_{i \neq j} \quad (\text{S } 1)$$

Solving for the eigenvalues we get:

$$\epsilon = \frac{1}{2}(\epsilon_{ii} + \epsilon_{jj}) \pm \frac{1}{2}\sqrt{(\epsilon_{ii} - \epsilon_{jj})^2 + 4V_{ij}^2} \quad (\text{S } 2)$$

If we expand this expression up to second order in V_{ij} we get:

$$\epsilon \approx \frac{1}{2}(\epsilon_{ii} + \epsilon_{jj}) \pm \left(\frac{1}{2}|\epsilon_{ii} - \epsilon_{jj}| + \frac{V_{ij}^2}{|\epsilon_{ii} - \epsilon_{jj}|} \right) \quad (\text{S } 3)$$

which leads to the following corrections to the states energies:

$$\begin{aligned} \tilde{\epsilon}_{ii} &= \epsilon_{ii} \pm \frac{V_{ij}^2}{|\epsilon_{ii} - \epsilon_{jj}|} \\ \tilde{\epsilon}_{jj} &= \epsilon_{jj} \pm \frac{V_{ij}^2}{|\epsilon_{ii} - \epsilon_{jj}|} \end{aligned} \quad (\text{S } 4)$$

and

$$\tilde{\epsilon}_{min} = \min \left(\epsilon_{ii} - \frac{V_{ij}^2}{|\epsilon_{ii} - \epsilon_{jj}|}, \epsilon_{jj} - \frac{V_{ij}^2}{|\epsilon_{ii} - \epsilon_{jj}|} \right) \quad (\text{S } 5)$$

This could be extended to all the elements and further corrections by the rest of the states to obtain the following general expression:

$$\tilde{\epsilon}_{min} = \min_i \left(\epsilon_{ii} - \sum_k \frac{V_{ik}^2}{|\epsilon_{ii} - \epsilon_{kk}|} \right) \quad (\text{S } 6)$$

This expression can hence be used to “gauge” for the lowest eigenvalue and by extension, to gauge for the energy difference. Note that this is similar to the Gershgorin method to have a lower/upper

¹Note that in the graph picture the interacting states will compose the nodes of a graph

bound for the eigenvalues, however, with a different expression for the “discs.” To avoid the problem of dividing by 0 when energies are similar, a tunable parameter $\delta > 0$ was added to the denominator leading to the following metric function f :

$$f = \min_i \left(\epsilon_{ii} - \sum_k \frac{V_{ik}^2}{|\epsilon_{ii} - \epsilon_{kk}| + \delta} \right) \quad (\text{S } 7)$$

If we want an expression without having to introduce a tunable parameter, one can rewrite Eq. S 2 as follows:

$$\epsilon = \epsilon_{ii} + \frac{1}{2}(\epsilon_{jj} - \epsilon_{ii}) \pm \frac{1}{2}\sqrt{(\epsilon_{jj} - \epsilon_{ii})^2 + 4V_{ij}^2} \quad (\text{S } 8)$$

which gives us a correction for ϵ_{ii} provided we pick the right sign on the third term. Let’s for now consider the following expression as the “correct” correction of ϵ_{ii} :

$$\tilde{\epsilon}_{ii} = \epsilon_{ii} + \frac{1}{2}(\epsilon_{jj} - \epsilon_{ii}) - \text{sign}(\epsilon_{jj} - \epsilon_{ii}) \frac{1}{2}\sqrt{(\epsilon_{jj} - \epsilon_{ii})^2 + 4V_{ij}^2} \quad (\text{S } 9)$$

In this case, if $\epsilon_{jj} - \epsilon_{ii} > 0$, the expression becomes:

$$\tilde{\epsilon}_{ii} = \epsilon_{ii} + \frac{1}{2}(\epsilon_{jj} - \epsilon_{ii}) - \frac{1}{2}\sqrt{(\epsilon_{jj} - \epsilon_{ii})^2 + 4V_{ij}^2} \quad (\text{S } 10)$$

which tends to ϵ_{ii} when V_{ij} tends to 0 since the second term is positive. On the other hand, when $\epsilon_{jj} - \epsilon_{ii} < 0$, the expression becomes:

$$\tilde{\epsilon}_{ii} = \epsilon_{ii} + \frac{1}{2}(\epsilon_{jj} - \epsilon_{ii}) + \frac{1}{2}\sqrt{(\epsilon_{jj} - \epsilon_{ii})^2 + 4V_{ij}^2} \quad (\text{S } 11)$$

which also tends to ϵ_{ii} when V_{ij} tends to 0 since the second term is negative.

We can now think about another expression for the metric gauging the energy difference which will read as follows:

$$g = \min_i \left(\epsilon_{ii} + \frac{1}{2} \sum_k \left((\epsilon_{ii} - \epsilon_{jj}) - \text{sign} \sqrt{(\epsilon_{ii} - \epsilon_{jj})^2 + 4V_{ij}^2} \right) \right) \quad (\text{S } 12)$$

which has the following equivalent expression²:

$$g = \min_i \left(\epsilon_{ii} + \frac{1}{2} \sum_k \left(|\epsilon_{ii} - \epsilon_{jj}| - \sqrt{(\epsilon_{ii} - \epsilon_{jj})^2 + 4V_{ij}^2} \right) \right) \quad (\text{S } 13)$$

Although Eq. S 13 is more rigorous since it does not possess any tunable parameter, it is also computationally more demanding since more operations need to be performed. This is an

²This can be easily proven considering the cases when $\epsilon_{jj} > \epsilon_{ii}$ and vice-versa

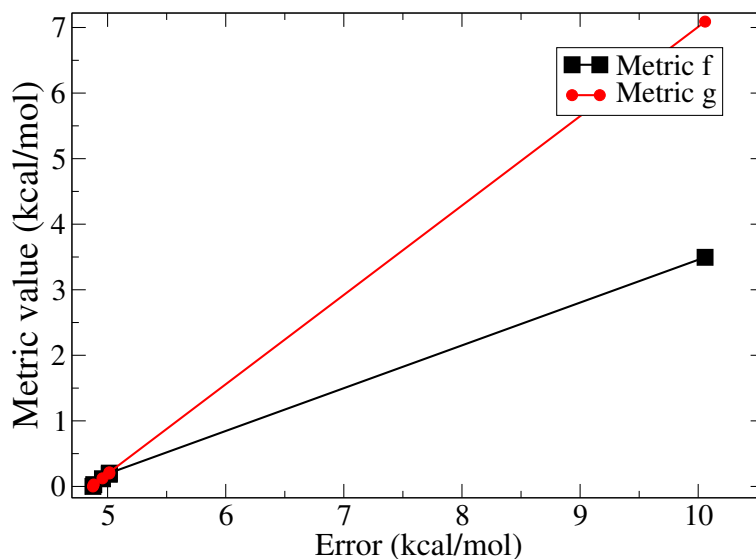


Figure S 2: Comparison between metric f and g in their ability to gauge the energy difference. The metric values were referred to the 2-clustering value to ease comparison. The system used here is a CO molecule FCI Hamiltonian matrix in the sto-3g basis set.

important point to consider since metric f is used as a gauge for the energy difference and it will need to be computed for every cluster at every k -clustering on a classical computer. This is hence one of the reasons for using metric f instead of g to gauge for the energy difference in this work.

Fig. S 2 shows a comparison of both metrics on the k -clustering of molecule CO using the FCI Hamiltonian matrix with sto-3g basis set. A parameter of $\delta = 1$ was used for computing metric f . We can clearly see that both metrics agree when the energy differences are low whereas metric f deviates from the linear trend as compared to metric g when the energy differences are higher. For the purpose of gauging the energy difference they are both equally suitable with the caveat that f is simpler to compute.

As was shown in the main manuscript, the metric shows both a good monotonicity and a good linearity for all the cases analyzed. It can determine the relevant cluster (without having to compute the energies for all the sub-graphs from the k -clustering). The sub-graph with the lowest gauge metric value will lead to the lowest energy (lower energy difference). Moreover, one of the advantages of this metric is that the formula is simple enough to understand what conditions for the cluster lead to the lowest energy. Here we have identified three main conditions:

- The lower the diagonal elements that are picked in the partition (relevant cluster), the lower will be the energy.
- The closer the energies of the nodes that belong to the partition that is picked, the lower will

Table S 11: Chemical accuracy from gauge space.

Molecule	Size	Gauge _{FCI} (Hartrees)	Gauge _{CL} (Hartrees)	Reduced Size	$E_{CL} - E_{FCI}$ (kcal/mol)
H ₂ 631G*	8	-1.86775811	0.00870209	4	5.56
H ₂ cc-PVDZ	22	-1.86093991	-1.85059347	12	6.49
H ₂ 6-311++G**	54	-1.87796529	-1.87382138	29	2.60
H ₂ aug-cc-PVQZ	1256	-1.88353813	-1.87335889	492	6.39
H ₂ O sto-3g	133	-83.91116169	-83.91106565	65	0.06
BH ₃ sto-3g	1250	-33.73576371	-33.73297808	625	1.75
			-33.73526023	321	0.31
			-130.5181132	1036	3.36
			-130.5127594	648	6.72
N ₂ sto-3g	1824	-130.5234671	-130.5180307	544	3.41
			-130.5230616	396	0.25
HCN (8,10) sto-3g	1576	-115.369203	-115.369203	792	1.25e-05
HCN (9,10) 6-31G*	4076	-117.3139781	-117.3063941	2110	4.76
C ₆ H ₆ (6,6) cc-PVQZ	104	-436.2190515	-436.2182797	52	0.48
C ₈ H ₁₀ N ₄ O ₂ (12,9) sto-3g	7056	-1584.331104	-1584.316145	3920	9.38

be the energy difference.

- The higher the coupling between nodes, the lower will be the energy difference.

This metric, together with the results presented, can tell us when the clustering method will work better. From the expression of f we can conclude that the clustering method will work better when the couplings between nodes are high as compared to the other conditions (proximity of the state energies in the relevant cluster, and the degree of how low are the individual energies of the relevant cluster).

The gauge can also be used to indicate whether a low energy cluster will be within chemical accuracy before diagonalization. The difference between the gauge of the original matrix and the gauge of the cluster will be within chemical accuracy (≤ 1.0 kcal/mol or $\leq 1.6\text{e-}03$ Hartrees). This is shown for a number of molecules in Table S 11. H₂ molecule results were not shown previously. The others were previously seen in Table S 1 and Table S 4. All molecule clusters that resulted in chemical accuracy were predicted correctly by using the gauge. Additionally, the gauge indicates when a cluster will not result in chemical accuracy. This could indicate that the original matrix could not be reduced using *Quantum Community Detection* or was already optimal. Further analysis is required to understand this fully.

References

1. Parrish, R. M. *et al.* Psi4 1.1: An open-source electronic structure program emphasizing automation, advanced libraries, and interoperability. *J. Chem. Theory Comput.* **13**, 3185–3197 (2017).