

Supporting Information

Boron-Engineered Interfacial Electronic States Orchestrate Layered Metal- π -Carbon Nitride Coupling for Intensified Nonradical Reactivity

Rui Ma^{a1}, Sai Bai^{a1}, Jiantao Tong^a, Jie Dong^b, Haoran Dong^b, Jingyun Fang^c, Jin Qian^{a*}

^a *Research & Development Institute in Shenzhen, School of Chemistry and Chemical Engineering, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, China*

^b *College of Environmental Science and Engineering, Hunan University, Changsha, Hunan 410082, China*

^c *Guangdong Provincial Key Laboratory of Environmental Pollution Control and Remediation Technology, School of Environmental Science and Engineering, Sun Yat-Sen University, Guangzhou 510275, PR China*

¹*These authors contributed equally to this work*

**Corresponding author: Jin Qian,*

E-mail address: qianjin@nwpu.edu.cn; qianjin131@yahoo.com.hk.

Text S1.

DFT Calculation Details

First-principles calculations were carried out using the Vienna Ab initio Simulation Package (VASP) [1,2] to elucidate the underlying reaction mechanisms. The projector augmented wave (PAW) method [3] was employed to describe the interaction between ionic cores and valence electrons. The exchange–correlation interactions were treated using the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional [4]. van der Waals interactions were accounted for using the DFT-D2 empirical correction method proposed by Grimme [5].

A kinetic energy cutoff of 500 eV was used for the plane-wave basis set. Brillouin zone sampling was performed using a $2 \times 2 \times 1$ Monkhorst–Pack k-point mesh. Electronic self-consistency was achieved when the total energy difference between iterations was less than 10^{-5} eV. All atomic positions were fully relaxed until the residual force on each atom was smaller than $0.05 \text{ eV} \cdot \text{Å}^{-1}$. To eliminate spurious interactions between periodic images, a vacuum spacing of 15 Å was introduced along the z-direction.

Fukui function has been widely used for prediction of reactive sites of electrophilic, nucleophilic, and radical attacking. Specifically, Fukui function is defined as:

Nucleophilic attack: $f^+(r) = \rho_{N+1}(r) - \rho_N(r)$ (S1)

Electrophilic attack: $f^-(r) = \rho_N(r) - \rho_{N-1}(r)$ (S2)

Radical attack: $f^0(r) = \frac{f^+(r) + f^-(r)}{2}$ (S3)

Where ρ_N is the atom charge population of atom k at corresponding state. The Fukui function contains relative information about different sites of one molecule.

Text S2

LCA analysis

In this study, we employed Simapro 9.4.0.1 and data Ecoinvent 3.8 to establish a model and quantified it using ReCiPe 2016 Midpoint (H) V1.07 / World (2010).

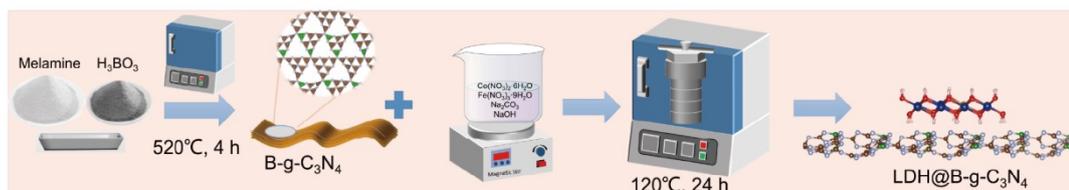


Figure S1. The synthetic procedure of LDH@BCN

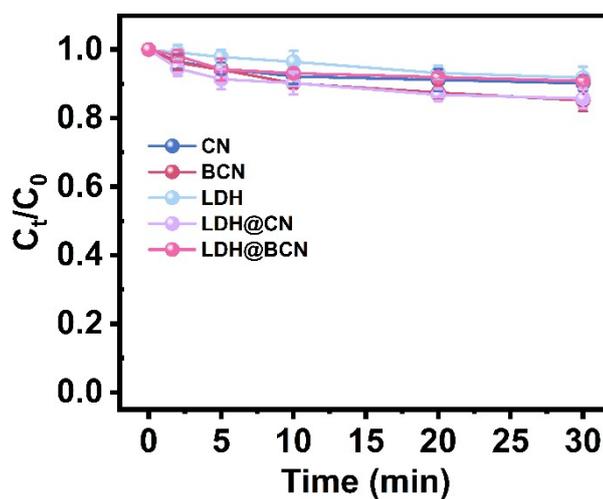


Figure S2. Adsorption performance of the as-prepared catalysts towards MMH.

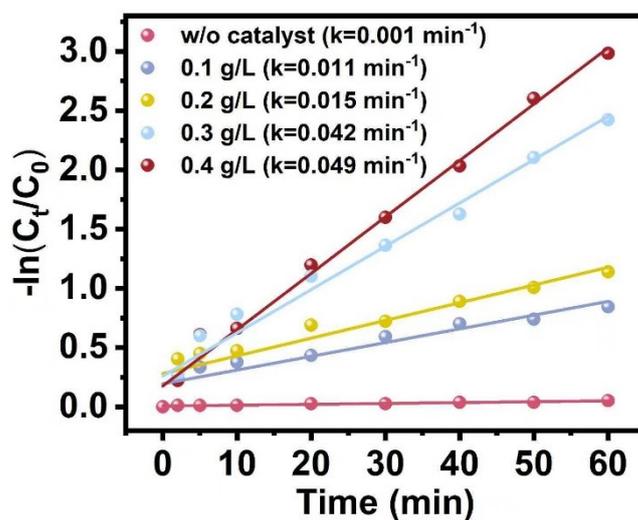


Figure S3. Pseudo-first-order kinetic plots in various catalyst dosage.

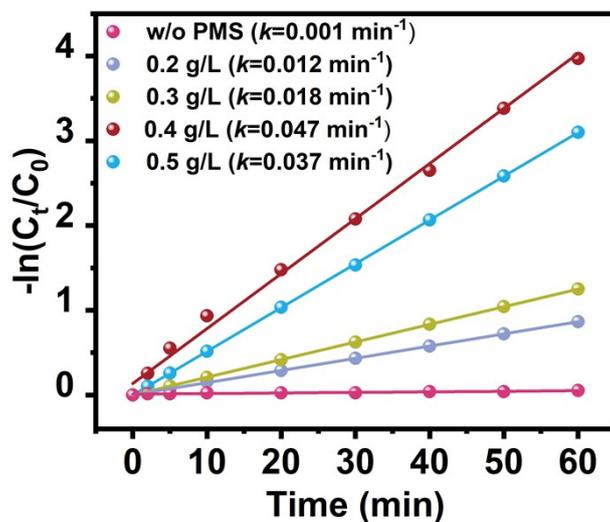


Figure S4. Pseudo-first-order kinetic plots in various PMS dosage.

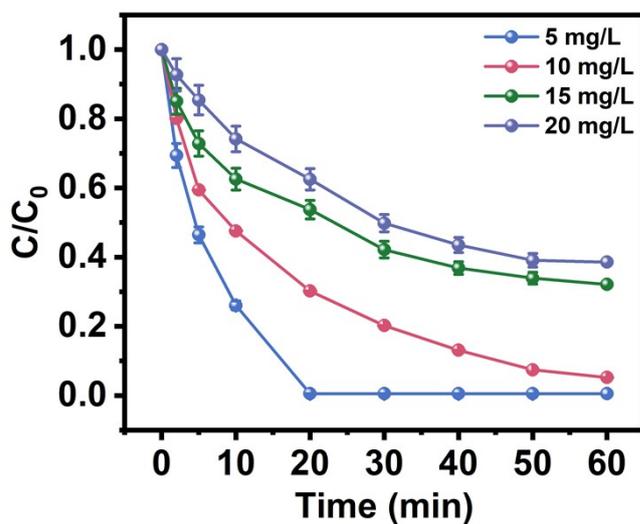


Figure S5. Effect of initial MMH concentration on degradation performance in the LDH@BCN/PMS system.

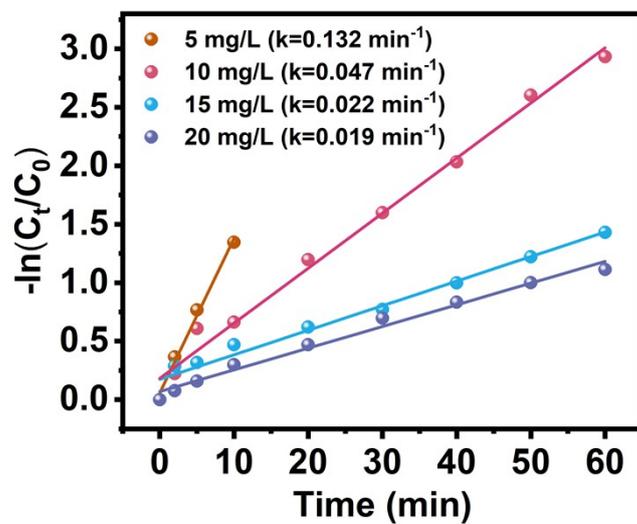


Figure S6. Pseudo-first-order kinetic plots in various MMH concentration.

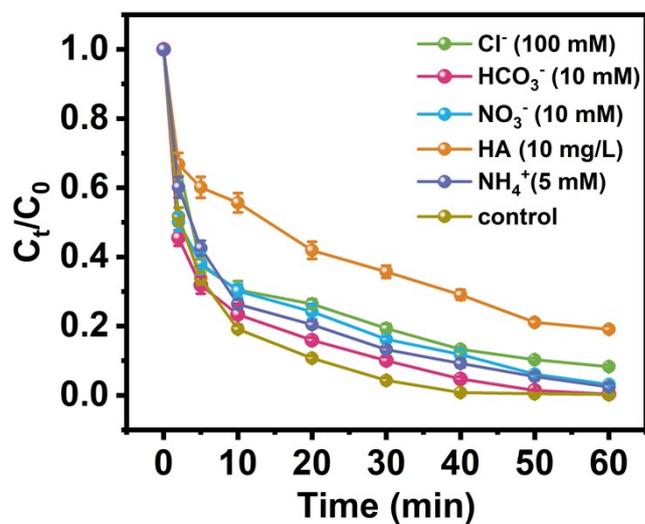


Figure S7. The impact of co-existing anions on MMH degradation.

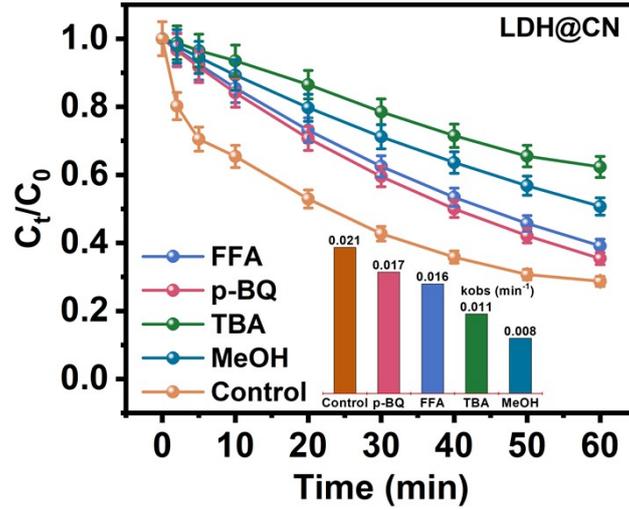


Figure S8. Quenching experiments for the LDH@CN system using various scavengers.

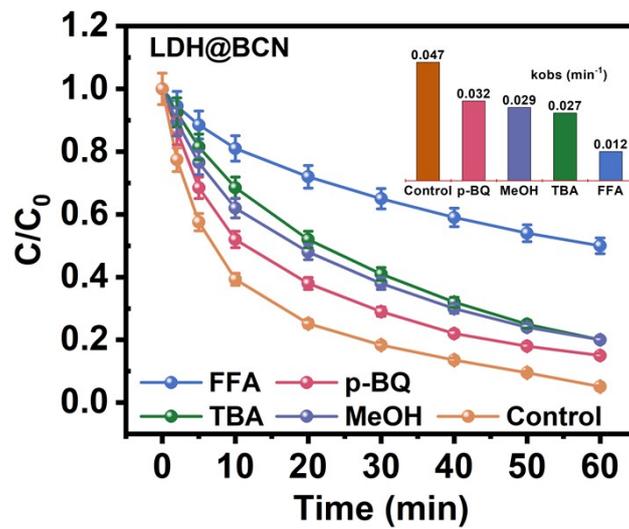


Figure S9. Quenching experiments for the LDH@BCN system using various scavengers.

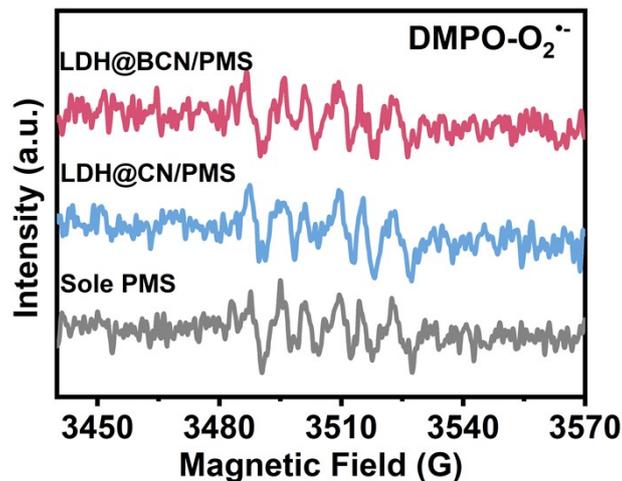


Figure S10. DMPO as a spin-trapping agent to detect superoxide radicals ($\text{DMPO-O}_2^{\cdot-}$) in different reaction systems.

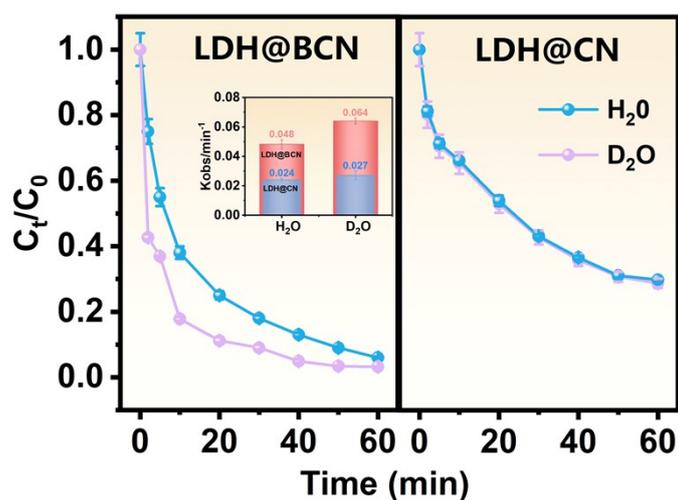


Figure S11. The influence of different solvent on MMH degradation.

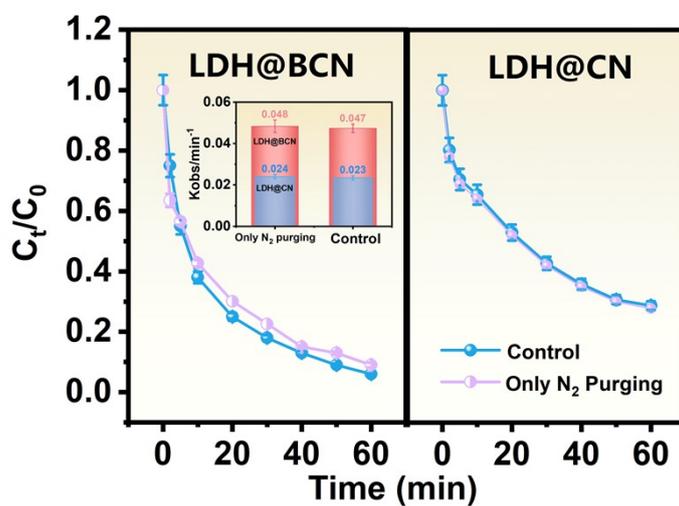


Figure S12. Degradation efficiency by LDH@BCN and LDH@CN with N_2 aerating.

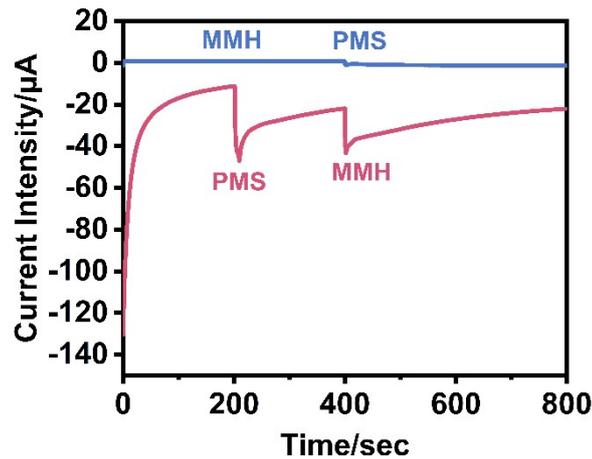


Figure S13. *i-t* curves of LDH@BCN coated glass carbon electrode (GCE) with PMS and MMH addition.

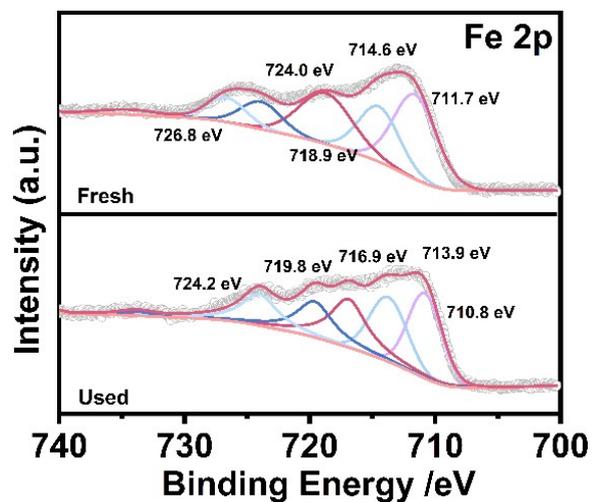


Figure S14. Fe 2p XPS spectra of LDH@BCN before and after reaction.

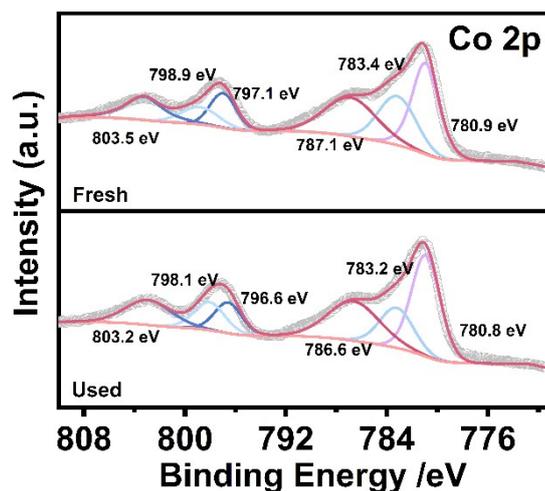


Figure S15. Co 2p XPS spectra of LDH@BCN before and after reaction.

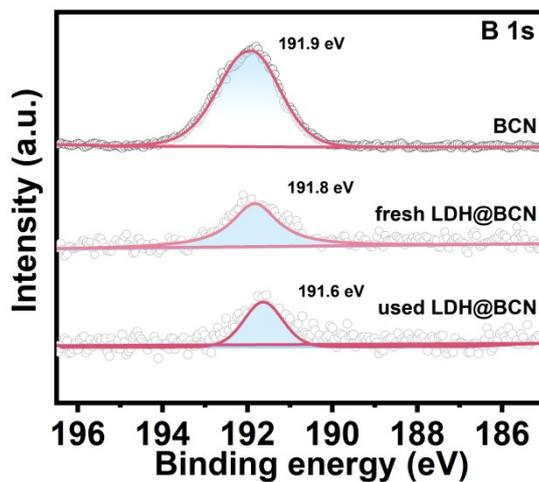


Figure S16. B 1s XPS spectra of as-prepared catalysts.

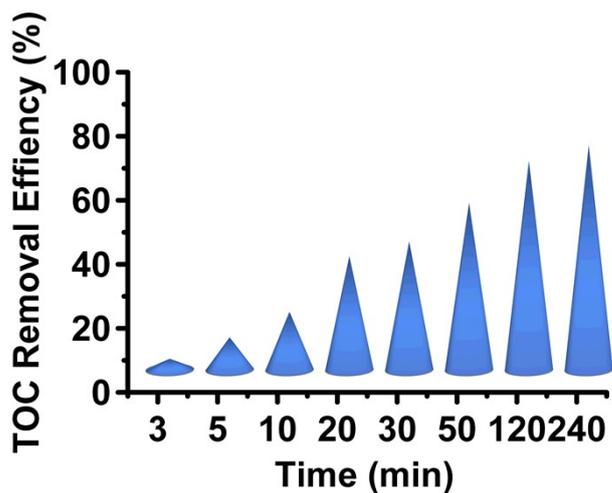


Figure S17. The TOC degradation efficiency in the LDH@BCN/PMS system.

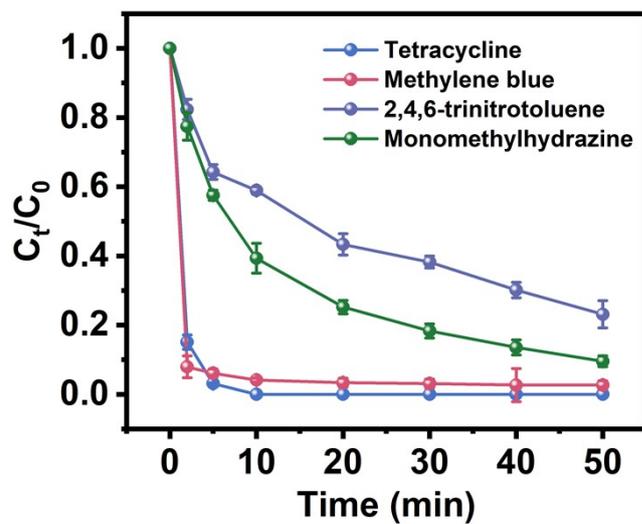


Figure S18. Degradation of different pollutant in LDH@BCN/PMS system.

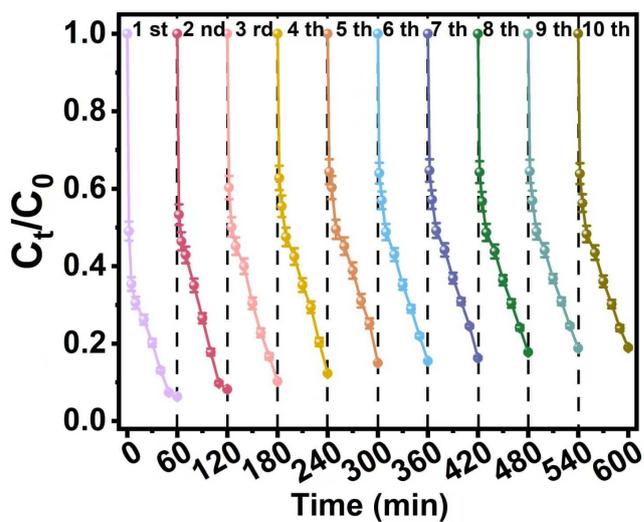


Figure S19. Cycling test in LDH@BCN/PMS system.

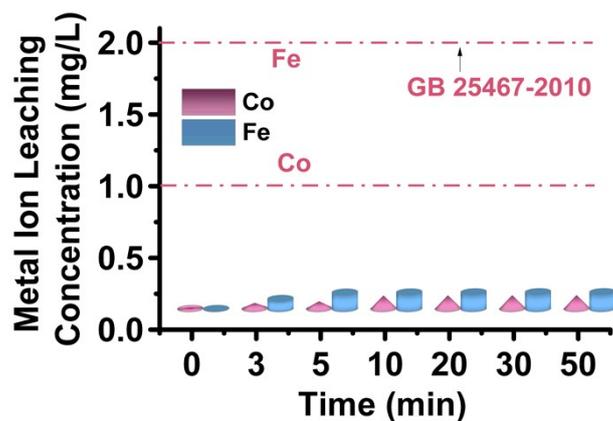


Figure S20. Time-dependent leaching concentrations of Fe and Co ions during the catalytic process.

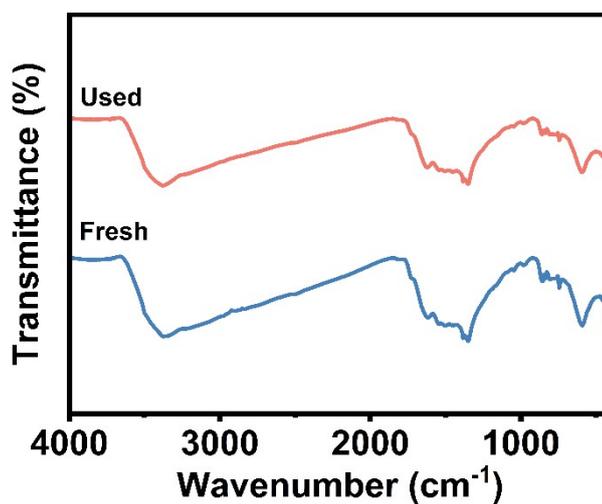


Figure S21. FT-IR spectra of LDH@BCN before and after catalytic reaction.

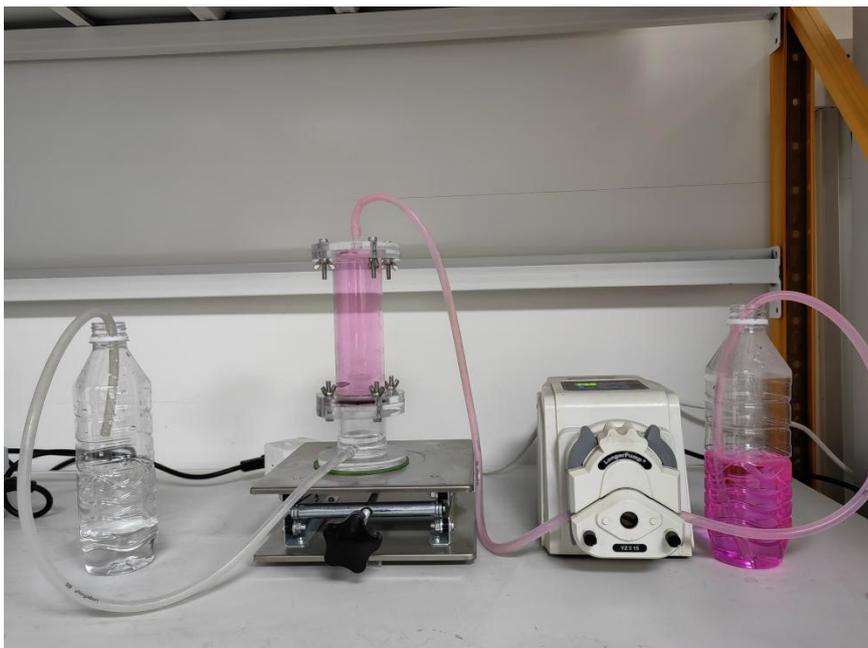


Figure S22. Photograph of the experimental setup used for continuous-flow dye simulation wastewater removal tests

Table S1 The content of transition metals in the as-prepared catalysts.

Sample	Co (mg g ⁻¹)	Fe (mg g ⁻¹)
LDH	300.18	220.30
LDH@BCN	92.52	60.41

Table S2. k values with various quenchers addition

	LDH@B-g-C ₃ N ₄	LDH@g-C ₃ N ₄
Control	0.047	0.021
p-BQ	0.042	0.019
MeOH	0.032	0.006
TBA	0.041	0.020
FFA	0.014	0.017

Table S3. Relative contribution of different ROS

	LDH@BCN/PMS system		LDH@CN/PMS system	
	α	β (%)	α	β (%)
$\bullet\text{OH}$	0.128	11.32	0.048	4.76
$\text{SO}_4^{\bullet-}$	0.191	16.98	0.667	66.67
$\text{O}_2^{\bullet-}$	0.106	9.43	0.095	9.52
$^1\text{O}_2$	0.702	62.27	0.190	19.05

Table S4. Input materials and energy required to treat 1 ton mono-methylhydrazine wastewater through different systems.

Treatment of 1 ton of mono-methylhydrazine wastewater	PMS Fenton system	LDH@CN/PMS system	LDH@BCN/PMS system
Reagents (g)			
Melamine	0	180	100
Na ₂ SO ₄	7000	0	0
Ethanol	0	5	5
NaOH	1500	0	27
H ₂ SO ₄	350	0	0
H ₃ BO ₃	0	0	100
Potassium peroxymonosulfate	1200	700	400
FeSO ₄ ·7H ₂ O	500	0	0
Co(NO ₃) ₂ ·6H ₂ O	0	126	72
Fe(NO ₃) ₃ ·9H ₂ O	0	122	70
Na ₂ CO ₃	0	26	15
NF	0	0	0
HCl	0	8.7	5
Energy (kWh)			
Power supply	2	0.35	0.2
Pump	4	0	0
Stirrer	8	7.0	4.0
Stirrer (reagents for the sludge treatment)	0.4	0	0
Pump (reagents for the sludge treatment)	2	0	0
Heat for catalyst preparation	0	22.0	22.0
Outputs streams(g)			
Generated sludge, dry base	1000	0	0
Exhausted catalyst	0	180	100

Table S5. Impact assessment for 1 kg Fe(NO₃)₃.

Impact category	Unit	Total	Iron(III) chloride, without water, in 14% iron solution state {GLO} market for Cut-off, S	Nitric acid, without water, in 50% solution state {RoW} market for nitric acid, without water, in 50% solution state Cut-off, S
Global warming	kg CO ₂ eq	1.967869	0.299552	1.668317
Stratospheric ozone depletion	kg CFC11 eq	3.39E-05	2.47E-07	3.36E-05
Ionizing radiation	kBq Co-60 eq	0.073893	0.061447	0.012446
Ozone formation, Human health	kg NO _x eq	0.002405	0.000962	0.001443
Fine particulate matter formation	kg PM2.5 eq	0.001894	0.000713	0.00118
Ozone formation, Terrestrial ecosystems	kg NO _x eq	0.002445	0.000976	0.001469
Terrestrial acidification	kg SO ₂ eq	0.00711	0.00156	0.00555
Freshwater eutrophication	kg P eq	0.000476	0.000235	0.000241
Marine eutrophication	kg N eq	2.88E-05	1.57E-05	1.31E-05
Terrestrial ecotoxicity	kg 1,4-DCB	7.404093	4.201315	3.202778
Freshwater ecotoxicity	kg 1,4-DCB	0.086836	0.048345	0.038491
Marine ecotoxicity	kg 1,4-DCB	0.113423	0.063014	0.050409
Human carcinogenic toxicity	kg 1,4-DCB	0.085216	0.044546	0.04067
Human non-carcinogenic toxicity	kg 1,4-DCB	1.607752	0.853462	0.75429
Land use	m ² a crop eq	0.038064	0.014262	0.023803
Mineral resource scarcity	kg Cu eq	0.006927	0.003665	0.003262
Fossil resource scarcity	kg oil eq	0.280614	0.077592	0.203021
Water consumption	m ³	0.019144	0.006274	0.01287
Calculation:	Analyze			
Results:	Impact assessment for 1 kg Fe(NO ₃) ₃			
Product:	1 kg Fe(NO ₃) ₃			
Method:	ReCiPe 2016 Midpoint (H) V1.07 / World (2010) H			

Indicator:	Characterization
Skip categories:	Never
Exclude infrastructure processes:	No
Exclude long-term emissions:	No
Sorted on item:	Impact category
Sort order:	Ascending

Table S6. Impact assessment for 1 kg Co(NO₃)₂.

Impact category	Unit	Total	Cobalt oxide {GLO} market for cobalt oxide Cut-off, S	Nitric acid, without water, in 50% solution state {RoW} market for nitric acid, without water, in 50% solution state Cut-off, S
Global warming	kg CO ₂ eq	14.39636	12.92501	1.471354
Stratospheric ozone depletion	kg CFC11 eq	4.35E-05	1.38E-05	2.97E-05
Ionizing radiation	kBq Co-60 eq	4.791255	4.780279	0.010977
Ozone formation, Human health	kg NO _x eq	0.034154	0.032882	0.001272
Fine particulate matter formation	kg PM2.5 eq	0.040758	0.039717	0.001041
Ozone formation, Terrestrial ecosystems	kg NO _x eq	0.034917	0.033621	0.001296
Terrestrial acidification	kg SO ₂ eq	0.116531	0.111637	0.004895
Freshwater eutrophication	kg P eq	0.008045	0.007833	0.000212
Marine eutrophication	kg N eq	0.002427	0.002415	1.15E-05
Terrestrial ecotoxicity	kg 1,4-DCB	710.6857	707.861	2.824655
Freshwater ecotoxicity	kg 1,4-DCB	3.046503	3.012557	0.033946
Marine ecotoxicity	kg 1,4-DCB	4.113739	4.069281	0.044458
Human carcinogenic toxicity	kg 1,4-DCB	1.414835	1.378966	0.035868
Human non-carcinogenic toxicity	kg 1,4-DCB	87.49094	86.8257	0.665238
Land use	m ² a crop eq	0.564583	0.54359	0.020992
Mineral resource scarcity	kg Cu eq	5.798263	5.795386	0.002877
Fossil resource scarcity	kg oil eq	4.880779	4.701726	0.179052
Water consumption	m ³	3.470987	3.459636	0.011351

Calculation:

Analyze

Results:

Impact assessment for 1 kg Co(NO₃)₂

Product:

1 kg Co(NO₃)₂

Method:

ReCiPe 2016 Midpoint (H) V1.07 / World (2010) H

Indicator:	Characterization
Skip categories:	Never
Exclude infrastructure processes:	No
Exclude long-term emissions:	No
Sorted on item:	Impact category
Sort order:	Ascending

Table S7. Impact assessment for the treatment of 1 ton of mono-methylhydrazine wastewater (PMS Fenton system).

		Na ₂ SO ₄	NaOH	H ₂ SO ₄	Potassium Peroxymonosulfate	FeSO ₄	Generated Sludge, dry base	Power Supply	Pump	Stirrer	Stirrer (reagents for the sludge treatment)	Pump (reagents for the sludge treatment)	
Global warming	kg CO ₂ eq	25.2343	4.116989	1.942735	0.057532	1.876215	0.140219	0.007318	2.084547	4.169095	8.338189	0.416909	2.084547
Stratospheric ozone depletion	kg CFC11 eq	8.61E-06	1.75E-06	2.09E-06	3.85E-08	1.10E-06	5.58E-08	2.62E-09	4.36E-07	8.72E-07	1.74E-06	8.72E-08	4.36E-07
Ionizing radiation	kBq Co-60 eq	0.868208	0.224143	0.215197	0.003814	0.153635	0.010361	0.000355	0.031793	0.063586	0.127172	0.006359	0.031793
Ozone formation, Human health	kg NO _x eq	0.073048	0.014501	0.005083	0.000355	0.005101	0.000494	9.05E-06	0.005793	0.011587	0.023173	0.001159	0.005793
Fine particulate matter formation	kg PM2.5 eq	0.052322	0.015124	0.004294	0.000809	0.00563	0.000351	7.33E-06	0.003184	0.006367	0.012735	0.000637	0.003184
Ozone formation, Terrestrial ecosystems	kg NO _x eq	0.073536	0.014719	0.005135	0.000362	0.005205	0.0005	9.22E-06	0.005806	0.011611	0.023222	0.001161	0.005806
Terrestrial acidification	kg SO ₂ eq	0.122744	0.040023	0.007477	0.002585	0.013765	0.000677	1.29E-05	0.007098	0.014196	0.028392	0.00142	0.007098
Freshwater eutrophication	kg P eq	0.008339	0.002755	0.001013	0.000111	0.001224	8.08E-05	1.54E-06	0.000384	0.000769	0.001538	7.69E-05	0.000384
Marine eutrophication	kg N eq	0.000621	0.000231	9.60E-05	2.93E-06	8.57E-05	4.20E-06	1.06E-07	2.45E-05	4.91E-05	9.81E-05	4.91E-06	2.45E-05
Terrestrial ecotoxicity	kg 1,4-	166.6759	104.6913	8.653382	8.942262	33.25451	1.738867	0.007117	1.144934	2.289868	4.579736	0.228987	1.144934

Freshwater ecotoxicity	DCB kg 1,4- DCB	1.6584 46	0.96402 6	0.1065 65	0.0795 29	0.32284	0.0184 57	0.00018 5	0.0203 47	0.0406 94	0.0813 87	0.00406 9	0.02034 7
Marine ecotoxicity	kg 1,4- DCB	2.1843 9	1.26167 5	0.1405 57	0.1037 39	0.423061	0.0241 22	0.00023 7	0.0281 71	0.0563 41	0.1126 82	0.00563 4	0.02817 1
Human carcinogenic toxicity	kg 1,4- DCB	1.3342 43	0.45439	0.1281 3	0.0156 79	0.199118	0.0175 87	0.00019 6	0.0633 1	0.1266 2	0.2532 41	0.01266 2	0.06331
Human non-carcinogenic toxicity	kg 1,4- DCB	36.780 92	18.6209 5	2.4008 86	1.5167	6.340467	0.3245 16	0.00291 4	0.9237 18	1.8474 36	3.6948 71	0.18474 4	0.92371 8
Land use	m ² a crop eq	0.7094 19	0.38648 9	0.0507 45	0.0054 07	0.056649	0.0060 58	0.00010 7	0.0248 74	0.0497 47	0.0994 94	0.00497 5	0.02487 4
Mineral resource scarcity	kg Cu eq	0.1099 42	0.07057 2	0.0066 07	0.0052 06	0.020858	0.0014 27	1.14E- 05	0.0006 42	0.0012 83	0.0025 66	0.00012 8	0.00064 2
Fossil resource scarcity	kg oil eq	5.5125 09	1.08777 1	0.4853 79	0.0225 12	0.547458	0.0361 41	0.00176	0.4062 79	0.8125 58	1.6251 16	0.08125 6	0.40627 9
Water consumption	m ³	0.2820 89	0.11998 3	0.0515 66	0.0048 11	0.06252	0.0008 8	2.82E- 05	0.0051 59	0.0103 17	0.0206 35	0.00103 2	0.00515 9

Calculation: Analyze
 Results: Impact assessment
 Product: Treatment of 1 ton of mono-methylhydrazine wastewater (PMS Fenton system).
 Method: ReCiPe 2016 Midpoint (H) V1.07 / World (2010) H
 Indicator: Characterization
 Skip categories: Never
 Exclude infrastructure processes: No
 Exclude long-term emissions: No
 Sorted on item: Impact category

Sort order:

Ascending

Table S8. Impact assessment for the treatment of 1 ton of mono-methylhydrazine wastewater (LDH@CN/PMS system).

		Melamine	Ethanol	Potassium Peroxymonosulfate	Fe(NO ₃) ₃	Co(NO ₃) ₂	Na ₂ CO ₃	HCl	Power Supply	Stirrer	Heat for catalyst preparation	Percentage Difference	
Global warming	kg CO ₂ eq	15.59966	1.129378	0.005587	1.094459	0.22472	0.22472	0.040802	0.007915	0.364796	7.295915	5.211368	62%
Stratospheric ozone depletion	kg CFC11 eq	5.44E-06	2.45E-07	5.12E-08	6.42E-07	8.93E-07	8.93E-07	1.45E-08	6.05E-09	7.63E-08	1.53E-06	1.09E-06	63%
Ionizing radiation	1 eq Co-60	0.338213	0.02348	0.000167	0.08962	0.011412	0.011412	0.00523	0.00057	0.005564	0.111276	0.079483	39%
Ozone formation, Human health	kg NO _x eq	0.04206	0.002245	2.22E-05	0.002975	0.00047	0.00047	8.36E-05	2.04E-05	0.001014	0.020277	0.014483	58%
Fine particulate matter formation	kg PM2.5 eq	0.025736	0.001705	1.62E-05	0.003284	0.000495	0.000495	6.13E-05	2.05E-05	0.000557	0.011143	0.007959	49%
Ozone formation, Terrestrial ecosystems	kg NO _x eq	0.042307	0.002335	2.32E-05	0.003036	0.000478	0.000478	8.68E-05	2.07E-05	0.001016	0.02032	0.014514	58%
Terrestrial acidification	kg SO ₂ eq	0.059597	0.004809	5.80E-05	0.008029	0.001326	0.001326	0.000176	4.14E-05	0.001242	0.024843	0.017745	49%
Freshwater eutrophication	kg P eq	0.003729	0.000356	2.14E-06	0.000714	0.000122	0.000122	3.43E-05	4.27E-06	6.73E-05	0.001346	0.000961	45%
Marine eutrophication	kg N eq	0.000279	3.87E-05	1.10E-05	5.00E-05	1.26E-05	1.26E-05	2.20E-06	3.50E-07	4.29E-06	8.59E-05	6.13E-05	45%
Terrestrial ecotoxicity	kg 1,4-DCB	35.06107	4.404344	0.020931	19.39847	1.902785	1.902785	0.279176	0.082617	0.200363	4.007269	2.862335	21%

Freshwater ecotoxicity	kg 1,4- DCB	0.4039 78	0.04449 2	0.00031 6	0.188323	0.0202 91	0.02029 1	0.00373 3	0.00089 1	0.0035 61	0.0712 14	0.050867	24%
Marine ecotoxicity	kg 1,4- DCB	0.5398 56	0.05916 6	0.00027 5	0.246786	0.0267 93	0.02679 3	0.00492 5	0.00116 4	0.0049 3	0.0985 97	0.070426	25%
Human carcinogenic toxicity	kg 1,4- DCB	0.6085 55	0.05085 4	0.00025 5	0.116152	0.0220 03	0.02200 3	0.00570 6	0.00064 1	0.0110 79	0.2215 86	0.158275	46%
Human non-carcinogenic toxicity	kg 1,4- DCB	11.355 02	0.97638 4	0.00885 4	3.698606	0.4385 92	0.43859 2	0.07236 8	0.01767	0.1616 51	3.2330 13	2.309295	31%
Land use	m ² a crop eq	0.2398 6	0.02537 2	0.00786 4	0.033045	0.0090 97	0.00909 7	0.00154 8	0.00024 3	0.0043 53	0.0870 58	0.062184	34%
Mineral resource scarcity	kg Cu eq	0.0377 71	0.00359 4	2.64E- 05	0.012167	0.0088 55	0.00885 5	0.00025 2	5.99E- 05	0.0001 12	0.0022 45	0.001604	34%
Fossil resource scarcity	kg oil eq	3.3355 16	0.38576 8	0.00117 1	0.31935	0.0527 12	0.05271 2	0.01291 5	0.00211 5	0.0710 99	1.4219 77	1.015698	61%
Water consumption	m ³	0.1258 34	0.04410 6	0.00079 2	0.03647	0.0049 43	0.00494 3	0.00255	0.00017 5	0.0009 03	0.0180 55	0.012897	45%

Calculation: Analyze
 Results: Impact assessment
 Product: Treatment of 1 ton of mono-methylhydrazine wastewater (LDH@CN/PMS system).
 Method: ReCiPe 2016 Midpoint (H) V1.07 / World (2010) H
 Indicator: Characterization
 Skip categories: Never
 Exclude infrastructure processes: No
 Exclude long-term emissions: No
 Sorted on item: Impact category
 Sort order: Ascending

Table S9. Impact assessment for the treatment of 1 ton of mono-methylhydrazine wastewater (LDH@BCN/PMS system).

		Melamine	Ethanol	NaOH	H ₃ BO ₃	Potassium Peroxymonosulfate	Co(N ₂ O ₃) ₂	Fe(N ₂ O ₃) ₃	Na ₂ CO ₃	HCl	Power Supply	Stirrer	Heat for catalyst preparation	Percentage Difference	
Global warming	kg CO ₂ eq	13.374	0.597906	0.005587	0.031084	0.079276	0.625405	0.093633	0.093633	0.02354	0.004549	0.208455	4.169095	7.441834	53%
Stratospheric ozone depletion	kg CFC11 eq	3.85E-06	1.30E-07	5.12E-08	3.34E-08	3.98E-08	3.67E-07	3.72E-07	3.72E-07	8.37E-09	3.48E-09	4.36E-08	8.72E-07	1.56E-06	45%
Ionizing radiation	kBq Co-60 eq	0.264423	0.012431	0.000167	0.003443	0.004049	0.051212	0.004755	0.004755	0.003018	0.000328	0.003179	0.063586	0.113501	30%
Ozone formation, Human health	kg NO _x eq	0.036816	0.001189	2.22E-05	8.13E-05	0.000524	0.0017	0.000196	0.000196	4.82E-05	1.17E-05	0.000579	0.011587	0.020682	50%
Fine particulate matter formation	kg PM2.5 eq	0.021802	0.000903	1.62E-05	6.87E-05	0.000427	0.001877	0.000206	0.000206	3.54E-05	1.18E-05	0.000318	0.006367	0.011366	42%
Ozone formation, Terrestrial ecosystems	kg NO _x eq	0.036984	0.001236	2.32E-05	8.22E-05	0.00053	0.001735	0.000199	0.000199	5.01E-05	1.19E-05	0.000581	0.011611	0.020726	50%
Terrestrial acidification	kg SO ₂ eq	0.04988	0.002546	5.80E-05	0.00012	0.001092	0.004588	0.000553	0.000553	0.000102	2.38E-05	0.00071	0.014196	0.02534	41%
Freshwater eutrophication	kg P eq	0.002971	0.000188	2.14E-06	1.62E-05	5.24E-05	0.000408	5.09E-05	5.09E-05	1.98E-05	2.45E-06	3.84E-05	0.000769	0.001373	36%

Marine eutrophication	kg N eq	0.000215	2.05E-05	1.10E-05	1.54E-06	2.04E-06	2.86E-05	5.25E-06	5.25E-06	1.27E-06	2.01E-07	2.45E-06	4.91E-05	8.76E-05	35%
Terrestrial ecotoxicity	kg 1,4-DCB	24.41486	2.331711	0.020931	0.138454	2.552953	11.08484	0.792827	0.792827	0.161063	0.047481	0.114493	2.289868	4.087415	15%
Freshwater ecotoxicity	kg 1,4-DCB	0.291519	0.023555	0.000316	0.001705	0.023389	0.107613	0.008454	0.008454	0.002154	0.000512	0.002035	0.040694	0.072638	18%
Marine ecotoxicity	kg 1,4-DCB	0.390984	0.031323	0.000275	0.002249	0.030551	0.14102	0.011164	0.011164	0.002841	0.000669	0.002817	0.056341	0.100569	18%
Human carcinogenic toxicity	kg 1,4-DCB	0.484809	0.026923	0.000255	0.00205	0.008243	0.066373	0.009168	0.009168	0.003292	0.000369	0.006331	0.12662	0.226017	36%
Human non-carcinogenic toxicity	kg 1,4-DCB	8.779652	0.516909	0.008854	0.038414	0.447106	2.113489	0.182747	0.182747	0.041751	0.010155	0.092372	1.847436	3.297673	24%
Land use	m ² a crop eq	0.194828	0.013432	0.007864	0.000812	0.00419	0.018883	0.00379	0.00379	0.000893	0.00014	0.002487	0.049747	0.088799	27%
Mineral resource scarcity	kg Cu eq	0.021759	0.001903	2.64E-05	0.000106	0.001575	0.006953	0.00369	0.00369	0.000145	3.44E-05	6.42E-05	0.001283	0.00229	20%
Fossil resource scarcity	kg oil eq	2.775626	0.20423	0.001171	0.007766	0.023778	0.182486	0.021963	0.021963	0.007451	0.001215	0.040628	0.812558	1.450416	50%
Water consumption	m ³	0.08237	0.02335	0.000792	0.000825	0.001623	0.02084	0.00206	0.00206	0.001471	0.0001	0.000516	0.010317	0.018416	29%

Calculation:

Analyze

Results:

Impact assessment

Product:

Treatment of 1 ton of mono-methylhydrazine wastewater (LDH@BCN/PMS system).

Method:

ReCiPe 2016 Midpoint (H) V1.07 / World (2010) H

Indicator:	Characterization
Skip categories:	Never
Exclude infrastructure processes:	No
Exclude long-term emissions:	No
Sorted on item:	Impact category
Sort order:	Ascending

Reference

- [1] Kresse, G. and Furthmüller, J. (1996) Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *Comput. Mater. Sci.* 6(1):0-50
- [2] Segall, M. D., Lindan, P. J. D., Probert, M. J., Pickard, C. J., Hasnip, P. J., Clark, S. J. and Payne, M. C. (2002) First-principles simulation: ideas, illustrations and the CASTEP code. *J. Phys.: Condens. Matter* 14(11):2717-2744
- [3] Blochl, P. E. (1994) Projector augmented-wave method. *Phys. Rev. B.* 50:17953-17979
- [4] Perdew J P , Burke K , Ernzerhof M . (1996) Generalized Gradient Approximation Made Simple. *Physical Review Letters*, 77(18):3865-3868.
- [5] Grimme, S. (2006) Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J. Comput. Chem.* 27(15):1787-1799