Supplementary Materials

Supplemental Experimental Procedures

Materials. Metal sources $Co(Ac)_2 \cdot 4H_2O$ and $Zn(Ac)_2 \cdot 2H_2O$ were purchased from Sinopharm Chemical Reagent Co., Ltd. Sodium alginate (SA) was purchased from Aladdin. Nitrogen gases were supplied in cylinders by Heli factory with 99.999% purity. Nafion® perfluorinated resin solution containing 5% Nafion® was purchased from Sigma-Aldrich. Ultrapure water with resistivity > 18 M Ω cm⁻¹ was used. Reduced graphene oxides was purchased from Institute of Coal Chemistry, Chinese Academy of Sciences.

Preparation of A-Co/r-GOs. Using a syringe, a 1 wt. % sodium alginate solution with 3 wt. % melamine and determined amounts of r-GOs (20% by mass) was added dropwise to a Zn^{2+}/Co^{2+} mixed aqueous solution (the molar ratio of $Zn^{2+}/Co^{2+}=100:1$, 50:1, 20:1, 10:1 and 3:1) with stirring to form hydrogels. After washed with distilled water, the as-prepared hydrogels were dehydrated via a freeze-drying process to obtain (Zn,Co)-Alg/r-GOs/melamine aerogels. Then the (Zn,Co)-Alg/r-GOs/melamine aerogels were placed in a tube furnace and heated in nitrogen atmosphere from room temperature to 550 °C where they were treated for 2 h, and subsequently heated to 900 °C and treated for 2 h. Finally, the as-obtained products were leached in 3 M HCl to remove cobalt NPs and dried in vacuum.

Preparation of contrast samples. For comparison, A-Co/r-GOs $(Zn_{10}Co_1)$ with different amounts of r-GO (10%–30% by mass), r-GOs (without the addition of Co), Co-NP/r-GOs (without the addition of Zn) and were synthesized using the similar method.

Characterizations. X-ray diffraction (XRD) was implemented by DX2700 (Dandong, China) operating with voltage 40 kV and current 30 mA equipped by Cu K α radiation (λ = 1.5418 Å). The morphology and structure of the samples were investigated by using a field emission scanning electron microscope (FESEM, JSM-7001F, JEOL, Tokyo, Japan) with an energy dispersive X-ray spectrometer (EDS). And transmission electron microscopy (TEM) and High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) were carried out by JEM-2100F (JEOL, Tokyo, Japan) with voltage of 200 kV. The specific surface area was calculated by the Brunauer-Emmett-Teller (BET) method with a relative pressure (P/P₀) range between 0.004 and 0.200. The pore size distribution plots were derived from the adsorption branch of the isotherms based on the BJH model. The chemical constitution was investigated by X-ray photoelectron spectroscopy (XPS) using an ESCALab250 electron

spectrometer (Thermo Scientific Corporation) with monochromatic 150 W Al Kα radiation. For X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS), the data collected at hard X-ray microanalysis (HXMA) beamline (BL), Canada Light Source (CLS). CLS storage ring operation at 250 mA mode, the beamline superconducting wiggler source was operated at1.7 T. The monochromatic X-ray beam was produced by using a double crystal Si(111) monochromator with its second crystal detuned by 50% at the end of the XAFS scan to reduce the high harmonic components in the X-ray beam. The beamline was configured in its focused mode with Rh mirrors (collimating and focusing mirrors) in the X-ray beam path. The experiment was performed in florescence mode by a 32 elements Ge detector, equipped with solar slits, arsenic filter (3 absorption length), and 4 layers of Al foil. The mono initial energy calibration was performed by using selenium elemental foil from EXAFS materials. During the experiment each individual XAFS scan was further calibrated by using the data in-step collected from the same Se foil, which was located between the two ion chamber detectors downstream of the sample. All three ion chamber detectors was filled with 100% He.

ORR test. For the electrochemical test, 6 mg of the catalyst was dispersed in the mixture of 50 µL of Nafion (5 wt. %) solution, 250 µL of ethanol, and 250 µL distilled water. Then a homogenous catalyst ink was obtained by an ultrasonic disperse method. 6 µL of the ink was pipetted onto a glassy carbon disk (0.1256 cm⁻²). Measurements were performed in a three-electrode equipped with a Pt counter electrode and a Ag/AgCl reference electrode. Cyclic voltammetry (CV) experiments with a sweep rate of 50 mV s⁻¹ were recorded in the potential range of 0 to -1.0 V vs. Ag/AgCl. Linear sweep voltammetry (LSV) was performed in N₂-saturated or O₂-saturated 0.1 M KOH. Current-voltage curves were recorded at a scan rate of 10 mv s⁻¹ under various electrode rotation rates (400, 625, 900, 1225, 1600, 2025, and 2500 rpm, respectively). The current density was normalized to the geometrical area and the measured potentials vs. Ag/AgCl were converted to a reversible hydrogen electrode (RHE) scale according to the following equation:

 $E_{RHE} = E_{Ag/AgCl} + 0.059 * pH + 0.1976$

The electron transfer number (n) of the sample was calculated from the ring current (IR) and disk current (ID) through the following equation:

$$n = \frac{4NI_D}{NI_D + I_R}$$

(N = 0.43) is the current collection efficiency of the Pt ring).

Aqueous Zinc-air batteries. For a primary aqueous zinc-air battery, the air electrode was prepared by uniformly coating the as-prepared catalyst ink onto carbon paper and then drying it at 80 °C for 2 h. The mass loading was 1.25 mg cm⁻² (0.25 mg cm⁻² for 20% Pt/C). A zinc

plate was used as the anode. Both electrodes were assembled into a home-built electrochemical battery with the electrolyte being 6 M KOH. Polarization data (V-*i*) were collected using linear sweep voltammetry at a scan rate of 10 mV s⁻¹.

The specific capacity normalized to the mass of consumed Zn was calculated based on the equation:

The specific capacity= Current *serve hours weight of consumed zinc

The gravimetric energy density normalized to the mass of consumed Zn was calculated based on the equation:

The gravimetric energy density= Current drain*serve hours*average discharge voltage weight of consumed zinc

The power densities of Zn-air batteries were calculated based on the equation:

 $P=U^*j$ (*P* is power densities of the battery (mW cm⁻²), *U* is the battery voltages (V), and *j* is current densities of the battery (mA cm⁻²)).

All-solid-state Zinc-air Batteries. The all solid-state Zn-air battery was fabricated by a polished zinc foil as anode, catalyst functioned Ni foam as cathode, gel polymer as solid electrolyte. The solid electrolyte was prepared as follow: 2 g polyvinyl alcohol (PVA) powder was added into 20 mL H₂O at 90 °C under stirring until the solution became uniform. Then, 5 mL 10 M KOH solution was added into the mixture. After being stirred for 1 h, the gel was poured onto a glass plate and freezed in a freezer at -20 °C for 3 h. The gel electrolyte was obtained after thawing at room temperature.

Density functional theory (DFT) calculations. The density functional theory (DFT) calculations were carried out using the Vienna ab Initio Simulation package (VASP).^{1, 2} The ion–electron interactions were described by the projector plane wave (PAW) approach. Electron exchange–correlations were represented by the functional of Perdew, Burke and Ernzerhof (PBE) of generalized gradient approximation (GGA).³ To ensure the convergence for total energy, all calculations were performed using a plane-wave cutoff energy of 400eV with Fermi-level smearing of 0.1eV and Monkhorst-Pack grid (3×3×1) was used for k-point sampling. Besides, the convergence threshold of energy and forces were set to be 1×10⁻⁵eV and 0.02eV/Å, respectively.

The overall ORR in alkaline environment is4:

 $\mathrm{O_2} + 2\mathrm{H_2O} + 4\mathrm{e^-} \rightarrow 4\mathrm{OH^-}$

The reaction is divided into four elementary steps⁵:

 $\begin{array}{ll} O_{2}(g) + 2H_{2}O(l) + 4e^{-} + * \to OH^{-} + OOH^{*} + H_{2}O(l) + 3e^{-} & (a) \\ OOH^{*} + OH^{-} + H_{2}O(l) + 3e^{-} \to 2OH^{-} + O^{*} + H_{2}O(l) + 2e^{-} & (b) \\ O^{*} + 2OH^{-} + H_{2}O(l) + 2e^{-} \to OH^{-} + OH^{*} + e^{-} & (c) \\ OH^{*} + 3OH^{-} + e^{-} \to 4OH^{-} + * & (d) \end{array}$

in which * implies the adsorption site.

For each step, the reaction free energy Δ Ga, Δ Gb, Δ Gc, and Δ Gd is is defined by following equation:⁴

$$\Delta \boldsymbol{G} = \Delta \boldsymbol{E} + \Delta \boldsymbol{Z} \boldsymbol{P} \boldsymbol{E} - \boldsymbol{T} \Delta \boldsymbol{S} - \Delta \boldsymbol{G}_{\!\boldsymbol{U}} + \Delta \boldsymbol{G}_{\!\boldsymbol{P} \!\boldsymbol{H}}$$

The ΔE , ΔZPE , and ΔS the different energy, zero-point energy, and entropy of the reaction, respectively. The ΔE is calculated by Density functional theory (DFT), ΔZPE , and ΔS are obtained from the values in ref. ^{5.6}

 $\Delta G_{pH} = -kT \ln 10 \times pH$

(pH=13 is used in the ORR calculation.)

$$\Delta G_{ii} = -eU$$

in which U is the potential measured at standard conditions (T = 298.15 K, P = 1bar, pH = 13).

The equilibrium potential (U_{ORR}^{eauil}) for ORR is obtained by the following equation:

$$U_{ORR}^{eauil} = 1.23 - kT \ln 10 \times pH = 0.461$$
 (V)

The barrier for ORR (E_{ORR}^{b}) at equilibrium potential is then obtained by the following equation,

 $E_{ORR}^{b} = \max \left\{ \Delta G_{a}, \Delta G_{b}, \Delta G_{c}, \Delta G_{d} \right\} + U_{ORR}^{equil} * e$ $= \max \left\{ \Delta G_{a}, \Delta G_{b}, \Delta G_{c}, \Delta G_{d} \right\} + 0.461$

Supplemental Data Items



Figure S1. The X-ray diffraction (XRD) patterns of Na-Alg, Co-Alg and Zn-Alg. Compared with Na-Alg. The broad diffraction peak of Co/Zn-Alg at 21.0° is ascribed to a typical "egg-box" structure in junction zones.^{7, 8}



Figure S2. XRD patterns of the samples with different Zn/Co ratio before acid leaching.



Figure S3. XRD patterns of Co-NP/r-GOs and the sample with Zn/Co=3:1 before and after acid leaching, respectively.



Figure S4. SEM (a) and TEM (b and c) images of the sample with Zn/Co=10:1 before acid leaching; (d) High resolution image of area marked in (b).



Figure S5. SEM (a), TEM (b) and magnified TEM (c-d) images of A-Co/r-GOs (Zn₁₀Co₁).



Figure S6. Four representative HAADF-STEM images of single-atom Co at different areas of A-Co/r-GOs ($Zn_{10}Co_1$).



Figure S7. EDX spectrum for A-Co/r-GOs ($Zn_{10}Co_1$).



Figure S8. (a) XPS survey; (b) High-resolution XPS spectra of C 1s of A-Co/r-GOs ($Zn_{10}Co_1$).



Figure S9. Raman spectroscopy of A-Co/r-GOs (Zn₁₀Co₁) obtained at different temperature (800, 900 and 950 °C).



Figure S10. Nitrogen adsorption-desorption isotherms and their corresponding pore size distributions of r-GOs (Zn) (a and d), A-Co/r-GOs ($Zn_{10}Co_1$) (b and f), Co-NP/r-GOs (Co) (c and g).



Figure S11. The corresponding EXAFS fitting curves for (a) Co foil and (b) Co-NP/rGOs.



Figure S12. XRD patterns of A-Ni/r-GOs and Ni-NP/r-GOs (a), A-Cu/r-GOs and Cu-NP/r-GOs (b).



Figure S13. HAADF-STEM images of the synthesized atomic Cu (a-b) and Ni (c-d) using sodium alginate as precursor.



Figure S14. (a) XPS survey; High-resolution XPS spectra of C 1s (b), N 1s (b) and Ni 2p (d) of A-Ni/r-GOs.



Figure S15. (a) XPS survey; High-resolution XPS spectra of C 1s (b), N 1s (b) and Cu 2p (d) of A-Cu/r-GOs.



Figure S16. Cu K-edge XANES (a) and FT-EXAFS spectra (b) for A-Cu/r-GOs; Ni K-edge XANES (c) and FT-EXAFS spectra (d) for A-Ni/r-GOs.



Figure S17. Thermogravimetric analysis of A-Co/r-GOs $(Zn_{10}Co_1)$ in air condition.



Figure S18. (a) LSV curves of A-Co/r-GOs ($Zn_{10}Co_1$) before and after 5000 potential cycles; (b) Long-term stability test of A-Co/r-GOs ($Zn_{10}Co_1$) and Pt/C.



Figure S19. HAADF-STEM images of atomic Co at different areas of A-Co/r-GOs ($Zn_{10}Co_1$) after stability test in O₂-saturated 0.1 M KOH.



Figure S20. LSVs at different rotation speeds (from 400 to 2500 rpm) of r-GOs (Zn) (a), A-Co/r-GOs (Zn₁₀₀Co₁) (b), A-Co/r-GOs (Zn₅₀Co₁) (c), A-Co/r-GOs (Zn₂₀Co₁) (d), A-Co/r-GOs (Zn₁₀Co₁) (e), A-Co/r-GOs (Zn₃Co₁) (f), and Co-NP/r-GO (g) in 0.1 M KOH aqueous solution saturated with O₂; (h) K-L plots for A-Co/r-GOs (Zn₁₀Co₁) at different potentials; (i) K-L plots obtained from LSVs of b-g at 0.5 V, separately.



Figure S21. (a) LSV curves of A-Co/r-GOs $(Zn_{10}Co_1)$ obtained at different temperature; (b) K-L plots and corresponding electron transfer numbers for these samples obtained from LSVs at 0.5 V; LSVs at different rotation speeds (from 400 to 2500 rpm) of the samples obtained at 850 (c) and 950 °C (d).



Figure S22. (a) LSV curves of A-Co/r-GOs $(Zn_{10}Co_1)$ with different amount of r-GO (by mass); (b) K-L plots and corresponding electron transfer numbers for these samples obtained from LSVs at 0.5 V; LSVs at different rotation speeds (from 400 to 2500 rpm) of the samples with 10 % (c) and 30 % r-GO (d).



Figure S23. (a) LSV curves of A-Co/r-GOs ($Zn_{10}Co_1$) and the sample before acid leaching; (b) LSVs at different rotation speeds (from 400 to 2500 rpm) of the sample before acid leaching.



Figure S24. The Tafel slope of A-Co/r-GOs ($Zn_{10}Co_1$) and the sample before acid leaching. The lower Tafel slope for A-Co/r-GOs ($Zn_{10}Co_1$) than that of the sample before acid leaching indicates the faster kinetics of A-Co/r-GOs ($Zn_{10}Co_1$).



Figure S25. (a) LSV curves at different rotation speeds (from 400 to 2500 rpm) of A-Co/r-GOs ($Zn_{10}Co_1$) in 0.5 M H₂SO₄. (b) The comparison of LSV curves of A-Co/r-GOs ($Zn_{10}Co_1$) and Pt/C



Figure S26. ORR polarization curves of A-Co/r-GOs ($Zn_{10}Co_1$) and 20 wt% Pt/C in O₂-saturated 6 M KOH solution.



Figure S27. Digital image of the home-made aqueous zinc-air battery.



Figure S28. The galvanostatic discharge curves of A-Co/r-GOs ($Zn_{10}Co_1$) and Pt/C-based ZABs at current densities of 1 and 5 mA cm⁻², respectively.



Figure S29. Mechanically recharged A-Co/r-GOs ($Zn_{10}Co_1$)-based ZAB at 50 mA cm⁻² after full-discharge process.

Sample	Path	Ν	σ2 (×10 ⁻³ Ų))	R (Å)	$\Delta E_0(eV)$
A-Co/r-GOs (Zn ₁₀ Co ₁)	Co-N	2.8	1.48	1.91	-8.081
	Co-C	1.2	0.29	1.76	-8.081
Co-NP/r-GOs	Co-Co	12	7.66	2.49	-5.961
Co foil	Co-Co	12	7.46	2.49	-6.614

 Table S1. EXAFS data fitting results of Samples.

Catalysts	Current	Voltage	Durablity	Current Density	Peak	Reference
	density	(V)		@ V=1.0 V	Power	
	(mA/cm²)			(mA/cm²)	Density	
A-Co/r-GOs	1	1 38	> 50 h	153.4	(mw/cm-)	This work
(Zn ₄₀ Co ₄)	5	1.30	> 50 h	155.4	225	THIS WORK
(=1110001)	Ū	1.01				
Co₃O₄/N-Graphene	10	~ 1.25	> 30 h	~75	190	ACS Appl. Mater.
						21138
	5	~ 1 22	22 h	~ 95	NI/A	Not Commun
COO/N-CNT	20	~ 1.35	22 II 12 h	~65	N/A	2013 4 1805
	20	1.2 V	12.11			2010,4.1000
Mn _x Co _{3−x} O₄/	20	~ 1.20	> 10 h	~150	N/A	Adv. Energy
N-Ketjenblack						<i>Mater.</i> 2016,
						1601052.
N,P, Fe tri-doped	1	~ 1.38	100 min	N/A	N/A	J. Mater. Chem. A,
porous carbon	10	~ 1.29	100 min			2016, 4, 8602.
NiO/CoN PINWs	5	1.37	N/A	~40	79.6	ACS Nano, 2017,
	10	1.29				112, 2275.
P,S-CNS	10	1.23 1.17	> 4 h	~80	198	ACS Nano, 2017,
	20					11, 347.
N-GCNT/FeCo-3	10	1.26	N/A	~50	97.6	Adv. Energy
	50	1.05				<i>Mater.</i> 2017, 7,
	100	0.82				1602420
S,N-Fe/N/C-CNT	N/A	N/A	N/A	~75	102.7	Angew. Chem. Int.
						<i>Ed.</i> 2017, 56, 610.
FeNC-850	50	1.1	22 h	~120	186	ACS Appl. Mater.
						Interfaces 2017, 9,
	25	1.07	40 h	200	224	4587.
Agnw-GA	25	~1.27	48 N	206	331	Adv. Funct. Mater.
	100	~1.25				1700041
CuCo₂O₄/N-CNTs	100	0.95	N/A	~70	95.5	Adv. Funct. Mater.
						2017, 27,
						1701833.
Co@NG-acid	10	1.37	14 h	255	350	Adv. Funct. Mater.
	50	1.33	4.5 h			2016, 26, 4397.
Fe ₃ C/Co(Fe)O _x @NC	5	1.37	30 h	177.5	231	ACS Appl. Mater.
NT	10	1.33	18 h			Interfaces 2017, 9,
						21216.

Table S2. A survey of primary ZABs with several key parameters extractedfrom the literatures.

Samples	Metal	Main precursors	Assessment of	Ref.
	loading		preparation process	
	0.0.0/			
A-Co/r-GOs	3.6 %	Sodium Alginate, Co(OAC) ₂ ,	High metal loading,	This work
(Zn ₁₀ Co ₁)		Zn(OAC) ₂ , r-GO	scale-up	
Co SAs/N-C(900)	4.3 %	ZIF-67	High metal loading,	Angew. Chem. Int. Ed.
			relative low yield	2016, 55, 10800.
S,N-Fe/N/C-CNT	0.8 %	FeCl ₃ , KSCN, CNT	Low metal loading,	Angew. Chem. Int. Ed.
			cannot realize scale-up	2017, 56, 610.
Fe-ISAs/CN	2.16 %	ZIF-8	High metal loading,	Angew. Chem. Int. Ed.
			relative low yield	2017, 56, 1.
Fe-N-SCCFs	3.9 %	Oleic acid, 1-octadecene,	High metal loading,	Nano Lett. 2017, 17,
		Sodium oleate, FeCl ₃ , hexane	complicated method	2003.
Ni SAs/N-C	1.53 %	ZIF-8	High metal loading,	J. Am. Chem. Soc.
			relative low yield	2017,139, 24, 8078.
Pt/TiN	0.35 %	TiN nanoparticles, H ₂ PtCl ₆ ·6H ₂ O	Low metal loading,	Angew. Chem. Int. Ed.
			cannot realize scale-up	2016, 55, 2058.
Co-N-C catalyst	3.6 %	Co(phen) ₂ (OAc) ₂ , Mg(OH) ₂ ,	High metal loading,	Chem. Sci. 2016, 7,
			cannot realize scale-up	5758.
lr₁/FeO _x	0.01 %	H ₂ IrCl ₆ , Fe(NO ₃) ₃ ,	Low metal loading,	J. Am. Chem. Soc.
			complicated method	2013, 135, 15314.
Co-NG	0.57 %	r-GO, CoCl ₂ ,	Low metal loading,	Nature Communi.
			cannot realize scale-up	2015, 6, 8668
ZnN _x /BP	0.3 %	Carbon black BP2000, HNO ₃ ,	Low metal loading, harsh	Adv. Funct. Mater.
		KOH, urea, Zn(OAC) ₂	method	2017, 27, 1700802.

Table S3. The metal loading and assessment of preparation process of A-Co/r-GOs and recently reported atomically dispersed catalysts.

Ref	E _{1/2}	electrolyte
Angew. Chem. Int. Ed. 2018, 57, 1856.	0.83 V vs. RHE	0.1 M KOH
J. Am. Chem. Soc. 2018, 140, 1737.	0.82 V vs. RHE	0.1 M KOH
Adv. Mater. 2017, 29, 1700707.	0.816V vs. RHE	0.1 M KOH
Angew. Chem. Int. Ed. 2017, 56, 1.	0.84 V vs.RHE	0.1 M KOH
Nano Lett. 2017, 17, 2003.	0.825 V vs.RHE	0.1 M KOH
Angew. Chem. Int. Ed. 2017, 56, 610.	0.82 V vs. RHE	0.1 M KOH
ACS Catal. 2017, 7, 6864.	0.848 V vs.RHE	0.1 M KOH
Angew. Chem. Int. Ed. 2016, 55, 10800.	0.811 V vs.RHE	0.1 M KOH
Adv. Mater. 2017, 29, 1703185.	0.81 V vs.RHE	0.1 M KOH
Adv. Energy Mater. 2017, 1700467.	0.8 V vs.RHE	0.1 M KOH
Adv. Mater. 2017, 29, 1701354.	0.82 V vs.RHE	0.1 M KOH
Adv. Mater. 2017, 29, 1700874.	0.82 V vs.RHE	0.1 M KOH
Adv. Mater. 2017, 29, 1606534.	0.841 V vs.RHE	0.1 M KOH
Angew. Chem. Int. Ed. 2017, 56, 13800.	0.83 V vs RHE	0.1 M KOH
This work	0.827 V vs RHE	0.1 M KOH

Table S4. A survey of the ORR activity $(E_{1/2})$ for commercial Pt/C extracted from the recent literatures.

References

- 1. L. Li, Y. Fang, R. Vreeker, I. Appelqvist, Biomacromolecules 2007, 8, 464.
- 2. Pawel Sikorski, Frode Mo, Gudmund Skjåk-Bræk, Bjørn T. Stokke, *Biomacromolecules*, **2007**, *8*, 2098.
- 3. H. Fei, J. Dong, Y. Feng, C. S. Allen, C. Wan, B. Volosskiy, M. Li, Z. Zhao, Y. Wang, H. Sun, P. An, W. Chen, Z. Guo, C. Lee, D. Chen, I. Shakir, M. Liu, T. Hu, Y. Li, A. I. Kirkland, X. Duan, Y. Huang, *Nature Catalysis*, **2018**, *1*, 63.
- 4. W. Chen, J. Pei, C. T. He, J. Wan, H. Ren, Y. Zhu, Y. Wang, J. Dong, S. Tian, W. C. Cheong, S. Lu, L. Zheng, X. Zheng, W. Yan, Z. Zhuang, C. Chen, Q. Peng, D. Wang and Y. Li, *Angew. Chem. Int. Ed.*, **2017**, *56*, 16086.
- 5. P. Yin, T. Yao, Y. Wu, L. Zheng, Y. Lin, W. Liu, H. Ju, J. Zhu, X. Hong, Z. Deng, G. Zhou, S. Wei and Y. Li, *Angew. Chem. Int. Ed.*, **2016**, *55*, 10800.
- 6. G. Kresse, J. Furthmüller, Phys. Rev. B 1996, 54, 11169.
- 7. G. Kresse, J. Furthmüller, Computational Mater. Sci. 1996, 6, 15.
- 8. J. P. John, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 1996, 77, 3865.