Ceramics Subcommittee Meeting Minutes Wednesday, 14 March 2018 International Centre Headquarters Conference Room A 1:00 p.m. – 2:00 p.m. W. Wong-Ng, Chairman

1. Call to Order

W. Wong-Ng

E. Antipov

The meeting was called to order at 1:05 pm by W. Wong-Ng

- Appointment of Minutes Secretary
 G. Kazimierczak was appointed as the minutes' secretary. Attendance list on record at headquarters.
- Approval of March 2017 Minutes
 W. Wong-Ng projected the minutes from March 2017, and the minutes were approved. Vote: 9/0/0
- 4. Review of Mission Statement

The Ceramics Subcommittee shall be responsible for (1) identifying ceramic compounds in the PDF, (2) organizing the ceramic subfile into minifiles according to their functions and properties, and (3) assuring the relevance and quality of the present and future data to meet the need of the user community.

W. Wong-Ng's presentation.

W. Wong-Ng asked if there were any objections to the term "minifiles." She indicated that someone suggested the term "chemical classes." There were no suggestions, and will continue to use the term "minifiles."

Organize the inorganic PDF into possible different properties. So far, there are currently seven or eight of them. Property Subfiles/Minifiles

5. Board of Directors Liaison Report

S. Misture stated there were no motions from the Subcommittee to report to the Board last year. Subfiles are critical to industry right now. If anyone has any ideas for motions, please write down a motion so it can be presented to the board so they know what the Subcommittee may be thinking about. It would help the Board to know what is going on.

6. Task Group Reports

(a)	Semiconductors	A. Davydov/M. Delgado
(b)	Bioceramics	Charlene Greenwood
(c)	Solar Materials	Y.C. Lan/N. King
		Y. Yan not present.
(d)	Thermoelectric Materials	W. Wong-Ng/Y. Yan
	123 from set 68 possible thermoelectric materials identified by	Y. Yan.

- (e) Superconductors
 - E. Antipov was not present. (See page 20.)
 - Uncertain how the Editor, at the time, assigned the materials to the SCM subfile. We want to make sure they are superconductor materials.
 - Reference/literature data needed to verify or remove compounds from the Superconductor SCM subfile.

Discussion:

- M. Leoni: If we don't have a motion, nobody will act.
- W. Wong-Ng: There are only six to eight patterns. Do we need a motion for that?
- M. Leoni: No motion, no action.
- Motion 1: W. Wong-Ng recommends to the Technical Committee that Headquarters' investigate if the following phases are superconductors based on literature references. NiAlSe , Al CeRh , CeGa Rh , Ce Ga Rh , CeGa Ru , Ga LaRu 3.7 10 2 2 2 2.6 10.4 1.7 1.3 3 2 There was no vote for the above motion.

(f)	Ionic Conductors	V.B. Nalbandyan /G. Subba Rao
(g)	Perovskites	L. Vasylechko
(h)	Hydrogen Storage Materials	I. Zavaliy
(i)	Ferroelectrics & Antiferroelectric	S. Ivanov/V. Nalbandyan/G.S. Rao
	No report.	
(i)	Cements	B. Scheetz

(j) Cements No report.

E. Pomerantseva

7. Technical Presentation - Battery Materials

E. Pomerantseva is the only one reviewing this subfile each year, and she invites others to join this subcommittee as her expertise is in synthesis, electric chemistry or new materials. It would be beneficial to have somebody with classic crystallographic expertise.

The Batteries Materials Subfile should be called Lithium Ionic electrode materials subfile, as the field has grown.

Motion 2: W. Wong-Ng recommends to the Technical Committee that headquarters expand the Battery Materials Subfile beyond Li-ion battery electrode materials.
 Motion passed. 14 Yes, 0 no, 0 Abstain.

8. New business Negative expansion coefficient materials (No discussion.)

C. Lind-Kovacs

- 9. New Members
- 10. Adjournment

Agenda

1. Call to order

- 2. Appointment of minutes secretary
- 3. Approval of the last meeting minutes
- 4. Review of Mission Statement
- 5. Board of Directors' Liaison Report
- 6. Task Group Reports:
- (a) Semiconductors
- (b) Bioceramics
- (c) Solar Materials
- (d) Thermoelectric Materials
- (e) Superconductors
- (f) Ionic Conductors
- (g) Perovskites
- (h) Hydrogen Storage Materials
- (i) Ferroelectrics & Antiferroelectrics
- (j) Cements
- 7. Technical Presentation Battery Materials
- 8. New business
 - New members

Negative expansion coefficient materials (Cora Lind-Kovacs)

9. Adjournment

W. Wong-Ng

Scott Misture

A. Davydov/M. Delgado Charlene Greenwood Y.C. Lan/N. King Y. Yan/W. Wong-Ng E. Antipov V.B. Nalbandyan /G. Subba Rao L. Vasylechko I. Zavaliy S. Ivanov/V. Nalbandyan/G.S. Rao B. Scheetz

Ekaterina Pomerantseva

Mission Statement

The Ceramics Subcommittee shall be responsible for (1) identifying ceramic compounds in the PDF, (2) organizing the ceramic subfile into minifiles according to their functions and properties, and (3) assuring the relevance and quality of the present and future data to meet the need of the user community.

Property Subfiles/Minifiles

Superconducting materials (SCM):

Elements, intermetallic alloys, or chemical compounds that will conduct electricity without resistance below a critical temperature (Tc).

Thermoelectric materials (TEM):

Thermoelectric materials (TEM: Commercially used thermoelectric materials (mostly semiconductors) are materials that have high Figures of Merit (ZT; materials with high Seebeck coefficient, high electrical conductivity and low thermal conductivity). The TEM code in the PDF will be used to represent thermoelectric materials that fall in a number of categories (Half-Heulsers, skutterudite, clathrates, pentatellurides, Di-chalcogenides, and layered-oxides, etc.). These materials have some or all of the associated properties (Seebeck coefficient, electrical conductivity or resistivity, thermal conductivity and figure of merit (ZT) available.)

Semiconducting materials (SEM):

Substances with electrical conductivity that is intermediate between those of conductors ($\sigma = 10^4 - 10^6 W^{-1} cm^{-1}$) and insulators ($\sigma = 10^{-12} - 10^{-10} W^{-1} cm^{-1}$). Conductivity semiconductors increases with temperature and in the presence of impurities.

"Hydrogen storage materials"

Intermetallic compounds with the capacity to absorb at least 0.5 H atoms per 1 metal atom (or weight H capacity of more than 1 wt.%)

Ionic conductors (ION):

Chemical compounds which electrical conduction is predominantly ionic (ionic transference number being in the excess of 0.95) with conductivity at least 10^{-5} σ /cm at temperatures within their solid-state existence range.

Ferroelectrics (FER):

Material that undergoes a phase transition from high-temperature phase that behaves as an ordinary dielectric to a low-temperature polar phase that has a spontaneous polarization whose direction can be switched by an applied field.

Battery materials (BAT):

Materials which have the following properties: 1) Capacity is expected to be at least 100 mAh/g; 2) For rechargeable batteries, the cyclability should be at least 10 cycles (No noticeable loss of the capacity should be observed for the first 10 cycles).

BioCeramics (BIO):

A ceramic used as a biomaterial. Biomaterials are substances, synthetic or natural in origin, which can be used as whole or as part of a system to treat, augment, or replace any tissue, organ, or function within the body. These inorganic, solid, crystalline materials must be highly biocompatible and antithrombogenic. They are used in prosthetics, bone implants, implant coatings, joint replacement, dental restoration and tissue engineering, including (but not limited to) the following systems: calcium phosphates (synthetic and natural); calcium sulfates; bioactive glasses and glass ceramics; titanium oxides; alumina; zirconia

W. Wong-Ng J. Yan J. A. Kaduk J. Martin G.Y. Liu Xian-Li Su S. H. Lapidus Q. Huang J. Anike R. Derbeshi Nacole King

NIST Wu Han University, China Illinois Institute of Technology NIST China University of Geosciences University of Michigan APS, ANL NIST Catholic University Morgan State University NIST/NRC post-doc

Thermoelectric Materials





Thomas Johann Seebeck (1770-1831)

John-Charles-Athanase Peltier (1785-1834)

Figure of Merits (ZT)



 $S = -V_{12}/\Delta T_{12}$ S-Seebeck Coeff Q = $\Pi \cdot I$ Π - Peltier Coeff

Seebeck Effect & Peltier Effect

Thermoelectric materials (TEM)

Thermoelectric materials (TEM: Commercially used thermoelectric materials (mostly semiconductors) are materials that have high Figures of Merit (ZT; materials with high Seebeck coefficient, high electrical conductivity and low thermal conductivity). The TEM code in the PDF will be used to represent thermoelectric materials that fall in a number of categories (Half-Heulsers, skutterudite, clathrates, pentatellurides, Di-chalcogenides, and layered-oxides, etc.). These materials have some or all of the associated properties (Seebeck coefficient, electrical conductivity or resistivity, thermal conductivity and figure of merit (ZT) available.)

Patterns prepared CaO-Gd₂O₃- CoO_x



Wong-Ng et al., SSS 72, 47-54

Samples/Patterns for Thermoelectric-related Materials Kaduk, Liu, Derbeshi, Anike, Yan, and Wong-Ng



Bi_{1-x} A_x Cu Se O (A=Ba, Ca)



R₂FeCoO₆

Set 68 Jack Yan (123)

Al3 Dv3 Fe Ge2 Al3 Co Ge2 Yb3 Al3 Ge2 Ni Yb3 Al4 Co Dy2 Ge2 Al4 Dy2 Ge2 Ni Nd0.5 Dv0.5 Fe O3 Nd0.5 Ho0.5 Fe O3 Sm0.5 Dy0.5 Fe O3 Sm0.5 Ho0.5 Fe O3 Gd0.5 Tb0.5 Fe O3 Gd0.5 Dv0.5 Fe O3 Gd0.5 Ho0.5 Fe O3 Eu Fe0.5 Al0.5 O3 Gd Fe0.5 Al0.5 O3 Dv Fe0.5 Al0.5 O3 Ho Fe0.5 Al0.5 O3 Y Fe0.5 Al0.5 O3 Pr Fe0.5 Ga0.5 O3 Nd Fe0.5 Ga0.5 O3 Sm Fe0.5 Ga0.5 O3 Sm Fe0.5 Cr0.5 O3 Al1.35 Co0.65 Er10

Al4 Co Ge2 Yb2 Al4 Ge2 Ni Yb2 Al2.9 Dv Sn0.1 Ir Sn0.45 Se1.55 **Tb Fe0.8 Mn0.2 O3 Tb Fe0.2 Mn0.8 O3** Nd (Co0.8 Ga0.2) O3 Nd (Co0.3 Ga0.7) O3 Eu (Co0.5 Ga0.5) O3 Eu (Co0.5 Ga0.5) O3 La0.5 Gd0.5 Mn O3 La0.7 Dy0.3 Mn O3 La0.3 Dv0.7 Mn O3 La0.9 Y0.1 Mn O3 Pr0.3 Nd0.7 Mn O3 Pr0.7 Nd0.3 Mn O3 Pr0.7 Y0.3 Mn O3 Nd0.5 Eu0.5 Mn O3 Sm0 5 Cd0 5 Mn O3 Nd (Co0.3 Ga0.7) O3 Gd (Co0.5 Ga0.5) O3 Er (Co0.5 Fe0.5)O3 Co (Sb0.95 Te0.05) S Co (Sb0.97 Te0.03) S Co (Sb0.99 Te0.01) S

Gd Fe0.5 Cr0.5 O3 Sm Fe0.5 Mn0.5 O3 Eu Fe0.5 Mn0.5 O3 Gd Fe0.8 Mn0.2 O3 Gd Fe0.2 Mn0.8 O3 Ho Fe0.8 Mn0.2 O3 Ho Fe0.3 Mn0.7 O3 Sm (Co0.5 Ga0.5) O3 Sm (Co0.5 Ga0.5) O3 Er (Co0.5 Fe0.5) O3 Y (Co0.5 Fe0.5) O3 Y (Co0.5 Fe0.5) O3 La0.7 Tb0.3 Mn O3 La0.3 Tb0.7 Mn O3 Pr0.3 Sm0.7 Mn O3 Pr0.7 Sm0.3 Mn O3 Nd0.5 Sm0.5 Mn O3 Nd0.5 Gd0.5 Mn O3 Sc3 Cu6.5 Al8.5 **Sc6 Cu22 Al14** Hf Ag Cu4 Ce3 V Ag7.25 Al24.75 Ce3 Mo Ag8.2 Al23.8 Gd3 Ta Ag9.5 Al22.65

Tb Fe0.8 Mn0.2 O3 Tb Fe0.2 Mn0.8 O3 Nd (Co0.8 Ga0.2) O3 Nd (Co0.3 Ga0.7) O3 Eu (Co0.5 Ga0.5) O3 Eu (Co0.5 Ga0.5) O3 La0.5 Gd0.5 Mn O3 La0.7 Dv0.3 Mn O3 La0.3 Dy0.7 Mn O3 La0.9 Y0.1 Mn O3 Pr0.3 Nd0.7 Mn O3 Pr0.7 Nd0.3 Mn O3 Pr0.7 Y0.3 Mn O3 Nd0.5 Eu0.5 Mn O3 Sm0 5 Gd0 5 Mn O3 Tb3 Co Al3 Ge2 Tb3 Ni Al3 Ge2 Lu2 Fe Al4 Ge2 La Ga Al Dv (Ga, Ge)3 Dy (Ga, Ge)3 Dy (Ga, Si)3 Sm5 Ga Sn2 Ti Call 5 Sil 5 Ir4 Pb Se8

Bi0.7 Ca0.3 Cu Se O Bi0.8 Ca0.2 Cu Se O Bi0.9 Ca0.1 Cu Se O Bi0.925Ca0.075CuSeO **Bi0.95 Ca0.05 Cu SeO** (Co0.95 Ni0.05) S (Co0.99 Ni0.01) SbS Bi0.8 Ba0.2 Cu SeO Bi0.85 Ba0.15 Cu SeO Bi0.875Ba0.125CuSeO (Co0.93 Ni0.07)SbS Co Sb (S0.93 Se0.07) Co Sb (S0.95 Se0.05) Co Sb (S0.97 Se0.03) Bi0.9 Ba0.1 Cu Se O Co Sb (S0.99 Se0.01) Co Sh S0 007 Sc Cu0.5 Al0.5 Lu3 Ni Al3 Ge2 Lu3 Co Al3 Ge2 Lu2 Co Al4 Ge2 Lu3 Fe Al3 Ge2 Y3 Mn Al3 Ge2 Er3 Mn Al3 Ge2 Y1.5 Ho1.5 Ni Al3 Ge2 **Dv3 Co0.5 Ni0.5 Al3 Ge2**

Summary ICDD Thermoelectric Property Data List (2010-17)

(Y Yan, J. Martin, X. L. Su, Wuhan Univ. of Technology, NIST, Michigan State Univ.)

AbSbTe ₂	BiCoZr	CoNbSn	$(\mathrm{Sr}_{0.67} \mathrm{Ba}_{1.33})\mathrm{Ba}_6(\mathrm{Al}_{14.10} \mathrm{Si}_{30.64})$	$(\mathrm{Ba}_4\mathrm{Ag}_3\mathrm{Ge}_{20}$
$Ba_8ga_{16}Ge_{30}$	CoSbZr	CoTiSb	$Ba_4Al_7Si_{15.5}$	$Ba_4Al_8Ge_{15}$
Ba _o Ga ₁₆ Si ₂₀	ErNiSb	ErPdBi	$Ba_4Al_8Si_{15}$	$Ba_4Au_3Ge_{20}$
Bi Se.	ErPdSb	Fe ₂ VA1	$Ba_4Cd_4Ge_{19}$	$\mathrm{Ba}_4\mathrm{Cu}_8\mathrm{P}_{15}$
$D_{12} S C_{3}$	HfCoSb	NiSbY	$Ba_4Ga_8Sn_{15}$	$\mathrm{Ba}_4\mathrm{Ga}_8\mathrm{Sn}_{15}$
$B_1 P_3$	NiSnHf	NiSnTi	$Ba_4In_8Ge_{15}$	Ba ₄ Ni ₃ Ge ₂₀
B1Sb	PtScSb	PtSnHf	Ba ₄ NiSi ₂₂	Ba ₄ Zn ₄ Ge ₁₉
CeFe ₄ Sb ₁₂	PtSnZr	cNiSb	$\mathrm{Ba}_{6}\mathrm{Ga}_{2.25}\mathrm{Ge}_{22.75}$	Ba ₆ Ge _{21.94} In _{3.06}
$CoSb_3$	ScPdSb	VFe ₂ Ga	$Ba_6Ge_{21}In_4$	Ba ₆ Ge ₂₄
FeSi	YPdSb	YPtSb	Ba ₆ Ge ₂₅	$\mathrm{Ba}_8\mathrm{Cu}_6\mathrm{Ge}_{40}$
GeTe	VFeSb	In _{0.05} CoSb ₃	Ba_8Ge_{43}	$Cs_8Cu_5Na_{16}Ge_{131}$
InAc	$Eu_{0.83}Fe_4Sb_{12}$	$Ca_{0.1}Co_4Sb_{12}$	$Cs_8Na_{16}Ge_{136}$	$Cs_8Na_{16}Si_{136}$
IIIAS	$Yb_{0.93}Fe4Sb_{12}$	YbFe ₄ Sb ₁₂	Eu ₈ Ga ₁₆ Ge ₃₀	$Ge_{15}P_8Te_4$
InP	$Ce_{0.1}Co_4Sb_{12}$	BaFe ₄ Sb ₁₂	$K_4Ga_4Sn_{19}$	Na_4Si_{23}
InSb	$CaFe_4Sb_{12}$	TlCoSb	$Si_{31.3}P_{14.7}Te_{7.35}$	Sn_3P_4
IrSb ₃	Cu ₂ Se	FeGa ₃	$Ba_{8-v}Sr_vAl_{14}Si_{32}$	YbZn ₂ Sb ₂
AgPb _m SbTe _{2+m}	MnSi _{1.75}	CuInTe ₂	$Bi_4O_4S_3$	YbMg ₂ Bi ₂
Mg ₂ Ge	CuGaTe ₂	CuInSe ₂	CeB ₆	YbCd ₂ Sb ₂
Mg ₂ Si	Ag ₂ S	Ag ₂ Se	CeTe ₂ Sb _x	$SrZn_2Sb_2$
Mg_2Sn	Ag ₂ Te	Bi_2S_3	$Ga_{3-x}In_{5+x}Sn_2O_{16}$	Mg_3Sb_2
$NaCo_2O_4$	$Ga_2 Te_3$	In_2Te_3	HfN	Mg_3Bi_2
PbS	In_3Te_4	BaSi ₂	LaFeAsO _{1-y}	$EuZn_2Sb_2$
PbSe	Ca ₂ Si	CdTe	SmNiC ₂	EuCd ₂ Sb ₂
PbTe	CoSi	Mg_3Sb_2	SrSi ₂	$CaZn_2Sb_2$
Sb_2Se_3	Cu ₂ GeSe ₃	AgCrSe ₂	$Yb_xEu_{1-x}Cd_2Sb_2$	$CaMg_2Bi_2$
Sb_2Te_3	Cu ₂ ZnSnSe ₄	Cu ₃ SbSe ₄	T1SbTe ₂	Ag ₈ GeTe ₆
SiGe	AgInTe ₂	Tl ₄ PbTe ₃	Zn_4Sb_3	$La_{3-x}Te_4$
SnTe	Tl ₄ SnTe ₃	Tl ₂ GeTe ₃	ZrNiSn	
$\mathrm{Sr}_8\mathrm{Ga}_{16}\mathrm{Ge}_{30}$	AgTlTe	AgGaTe ₂		

SmNiC₂

Chemical name: Samarium Nickel Dicarbide

Chemical formula: SmNiC₂

Crystal structure at RT: Amm2, a = 3.6970 Å, b = 4.5290 Å, c = 6.0960 Å

Powder Patterns: 98-016-9802, 98-016-8564

Single-crystalline material of $SmNiC_2$ has orthorhombic $CeNiC_2$ structure type with space group Amm2 and lattice parameters a=3.7037(3), b=4.5279(2), and c=6.0947(4) Å at room temperature, in agreement with previous studies (Fig.1). [1,2]







Fig.2 Thermoelectric properties of SmNiC2

(TMS) Thermoelectric Diffraction Data-ICDD/NIST

2018 TMS meeting (Phoenix, AZ)

NIST-ICDD Standard reference materials & Data

- SRM
 - LT Seebeck Coefficient-Bi₂Te₃
 - HT Seebeck Coefficient- Si_{0.8}Ge_{0.2}

• Reference Powder diffraction Data

- Collaboration with ICDD
- ICDD Publishes data since 1950's
- Powder Diffraction file (PDF)
 For Phase ID and characterization
- Ceramics subcommittee Thermoelectric task group
 - 200 patterns
 - 13 (Bi,A)CuSeO patterns
 - 140 property data sheets
- Welcome your contribution to the PDF

International Centre for Diffraction Data



- Scientific organization and publishing house – Powder Diffraction File (PDF) (≈400,000 inorganic, 526126 organic)
- 300 members
- Field of powder diffraction & related disciplines
- Grant-in-Aid: high quality powder diffraction data contact: DelCasale@icdd.com

Superconductor SCM subfile (Set 68)

SCM: $C_{1.12}H_{4.48}Fe_{2}Li_{0.34}N_{1.12}Se_{2}$ and $C_{1.12}H_{4.48}Fe_{2.08}Li_{0.34}N_{1.12}Se_{2}$ (Fe,Se – based superconductors)

I could not find the reference data for the following compounds (their patterns were marked by the ICDD staff as belonging to the SCM subfile). I am not sure that this is the correct assignment. It is necessary to find literature data for these compounds otherwise the SCM flag should be removed: NiAlSe_{3.7}, Al₁₀CeRh₂, CeGa₂Rh₂, Ce_{2.6}Ga_{10.4}Rh, CeGa_{1.7}Ru_{1.3}, Ga₃LaRu₂

Solar Materials

Physical Properties of Solar Materials (2017)

Nacole B. King and Yucheng Lan



Focusing on semiconducting elements and III-V compounds in 2017

Solar Materials



Solar Materials

III-V Nitrides:

Indium Nitride (InN) Gallium Nitride (GaN) Boron Nitride (BN)

III-V Phosphides:

Gallium Phosphide (GaP) Indium Gallium Phosphide (InGaP)

II-VI Compounds

Cadmium Sulfide (CdS) Cadmium Selenide (CdSe)

Others:

Copper Zinc Tin Sulfide (CZTS)



Solar Materials (Data sheets)

Finished Before 2017

(1) Se
(2) Cu2O
(3) Si
(4) GaAs
(5) InP
(6) CIGS
(7) CdTe
(8) GaSb
(9) Ge
(10) CIS: CuInSe2

FY2007-2008

- 1. Indium Nitride (InN)
- 2. Gallium Nitride (GaN)
- 3. Boron Nitride (BN)
- 4. Gallium Phosphide (GaP)
- 5. Indium Gallium Phosphide (InGaP)
- 6. Copper Zinc Tin Sulfide (CZTS)
- 7. Cadmium Sulfide (CdS)
- 8. Cadmium Selenide (CdSe)
- 9. Diamond (C)
- 10.carbon nanotube (C)

Solar Materials (Data sheets)

CdS₂

Photovoltaic Properties of Hexagonal Cadmium Sulfide

Chemical name: Cadmium Sulfide Chemical formula: CdS Crystal structure at RT: P63mc, a = 4.136 Å, c = 6.713 Å, Z = 2 Powder Patterns: 41-1049, 70-2553

Wurtzite cadmium sulfide was discovered in 1840, also named as greenockite after its discover Load Greenock. The material has been widely studied since the 1950s due to its applications in photovoltaic and luminescent devices.

Hexagonal CdS is a direct band gap semiconductor. Room temperature energy band gap of CdS crystals is 2.43 eV measured from natural logarithm of the resistance with the inverse of the temperature [2]. The value is close to that (2.37 eV) measured from absorption coefficient [1].

The transmittance of CdS crystals was measured [3]. CdS crystals were cut into 1 X 1 cm plates having the c axis lying in the plane of the plates. The wavelength-dependent transmittance was measured on a 0.106-cm-thick CdS crystal, from the visible through the near infrared. The material is transparent in the solar spectral region and its transmittance decreases rapidly for wavelengths greater than 10 μ m. The upper limit of about 16 μ m enable its application as infrared wave plates. The sharp increase of transmittance around 510 nm, then smoothly until 700 -900 nm, has been observed in crystals grown by vertical pulling method [4] with non-stoichiometeric crystals, by physical vapor transport [5]. Typically it has a peak sensitivity wavelength of about 560 nm to 600 nm in the visible spectral range. Therefore, cadmium sulphide has been commonly used to detect light in the infra-red range as photoconductive cells because its spectral response curve closely matches that of the human eye.

Photovoltaic behavior of CdS was first reported in 1954 [6]. The CdS photovoltaic cells were fabricated by applying the indium base electrode and silver counter electrode on opposite faces of a vapor-phase-grown CdS crystal approximately 3 mm thick. An open-circuit voltage of 0.4 V was measured and a short-circuit current of 15 mA // cm² was measured in direct sunlight. The photovoltaic effect was also observed in pressed fired CdS powders [6, 7].

Later, CdS metal Schottky barriers have been investigated [20] for photovoltaic applications, including Fe, Ag, Cu, Ni, and Te etc. CdS-Al Schottky junctions [8, 21, 22] and Au-CdS Schottky junctions [9] were also reported recently. PV effects were observed in these Schottky devices. In a modern CdS Schottky solar cell, CdS is usually deposited on a substrates, followed by a metal deposition on the *n*-type CdS film. Table 1 lists some PV properties of Schottky barrier-based PV cells.



FIG. 1. I-V characteristics of CdS-p-Si cells [10]. Curve 1: un-doped CdS p-type Si cell; Curve 2: Cl-doped CdS p-type Si cell.



FIG. 2. Photovoltaic spectral response of CdS-p-Si junctions [10]. Thickness of CdS films is 0.4 microns (curve 1) and 1.5 microns (curve 2). Efficiency: 5.5 %.

Besides bulk materials. CdS films have been fabricated as solar cells. CdS was first deposited to Si crystalline substrates [10] to form heterojunctions or Schottky barriers as PV cells, or onto Si nanopillats to form heterojunctions [12, 23]. A high energy conversion efficiency of 1.83 % was achieved recently [12]. More detailed information of CdS-Si solar cells is listed in Table 1. I-V characteristics and photovoltaic spectral response of planar CdS/Si solar cells are shown in Figure 1 and Figure 2 respectively.



FIG. 3. I-V characteristics of a cell with Cu-doped CdS / non-doped CdS structure [24]. Inset of the figure shows the structure.

As-prepared CdS thin films are usually *n*-type and the conductivity is controlled by deviation from the stoichiometry *p*-type CdS films can be generated from Cu doping [24,27]. Through Cu-doping, homojunction CdS solar cells have been fabricated by spray pyrolisis [11, 24]. In a typical homojunction CdS solar cells, cadmium sulfide thin films were prepared by spray pyrolisis over SAO2 coated glass substrates. Thickness of the CdS film was about 1.5 um and the type of conductivity of as-prepared films was *n*-type. High pure copper was then deposited on the as-prepared *n*-CdS films using vacuum evaporation at room temperature. The produced films were finnally annealed to diffuse Cu into CdS layers to form p-type CdS layers. Figure 3 and shows I-V characteristics and photovoltaic spectral response curve of *n*-CdS Cu-doped CdS homojunction solar cells respectively. The detailed values are listed in Table 1.

Solar Materials (Set 68)

	A	В	C	D	E	F	G	H
1	PDFID	Formula	Name	I.	0	М	Alloy	SubFileId
2	103854	Cu6 Sn5	Copper Tin	1	0	0	1	SOL
3	104615	TI2 S	Thallium Sulfide	1	0	1	0	SOL
4	104628	Ba Fe O2	Barium Iron Oxide	1	0	0	0	SOL
5	104629	Sr0.1 Ba0.9 Fe O2	Barium Strontium Iron Oxid	1	0	0	0	SOL
6	104630	Sr0.2 Ba0.8 Fe O2	Barium Strontium Iron Oxid	1	0	0	0	SOL
7	104631	Sr0.3 Ba0.7 Fe O2	Barium Strontium Iron Oxid	1	0	0	0	SOL
8	104632	Sr0.4 Ba0.7 Fe O2	Barium Strontium Iron Oxid	1	0	0	0	SOL
9	104633	Sr0.5 Ba0.5 Fe O2	Barium Strontium Iron Oxid	1	0	0	0	SOL
10	104634	Sr0.6 Ba0.4 Fe O2	Barium Strontium Iron Oxid	1	0	0	0	SOL
11	106094	Ba Fe12 O19	Barium Iron Oxide	1	0	0	0	CER,SOL
12	106095	Ba Fe11.4 (Ni0.5 Ti0.5)0.6	Barium Nickel Iron Titaniun	1	0	0	0	CER,SOL
13	106096	Ba Fe10.8 (Ni0.5 Ti0.5)1.2	Barium Nickel Iron Titaniun	1	0	0	0	CER,SOL
14	106097	Ba Fe10.2 (Ni0.5 Ti0.5)1.8	Barium Nickel Iron Titaniun	1	0	0	0	CER,SOL
15	106098	Ba Fe10 (Ni0.5 Ti0.5)2 O19	Barium Nickel Iron Titaniun	1	0	0	0	CER,SOL
16	106099	Ba Fe9.5 (Ni0.5 Ti0.5)2.5 O	Barium Nickel Iron Titaniun	1	0	0	0	CER,SOL
17	106487	Se	Selenium	1	0	0	1	SOL
18	106635	Nb O2	Niobium Oxide	1	0	0	1	BAT,SOL
19	106660	Cs In Ge S4	Cesium Germanium Indium	1	0	0	1	CER,SOL
20	106661	Cs In Ge S4	Cesium Germanium Indium	1	0	0	1	CER,SOL
21	106662	Cs In Sn S4	Cesium Indium Sulfide Tin	1	0	0	1	CER,SOL
22	106663	K In Ge S4	Germanium Indium Potassi	1	0	0	1	CER,SOL
23	106664	Li In Sn S4	Indium Lithium Sulfide Tin	1	0	0	1	CER,SOL
24	106667	Rb In Sn S4	Indium Rubidium Tin Sulfid	1	0	0	1	CER,SOL
25	106895	Cu Se2	Copper Selenide	1	0	1	1	SOL
26	106950	Ag2 S	Silver Sulfide	1	0	0	1	SOL
27	106951	Ag1.93 S	Silver Sulfide	1	0	0	1	SOL
28	107106	In2 O3	Indium Oxide	1	0	0	1	SOL

Ionic Conductors

V.B. Nalbandyan and G.V. Subba Rao

List of entries for Set 68 of the PDF has been reviewed:

- 12 previous ION marks are wrong and two more are doubtful (no data found)
- 14 previous ION marks are correct
- 2 new ION entries are identified
- One new BAT entry and one new FER entry are identified.

Perovskites

Leonid Vasylechko's activities

- 1. Set 68 was reviewed and **119** patterns of the perovskite phases were identified;
- Regular submission of experimental patterns through Grant-in-Aid Program. Totally, more than 660 experimental patterns were submitted since 2002, in particular about 570 patterns of the perovskite and perovskite-related phases.
- 3. During the last year property sheets were submitted for **30** materials

"Thermal Expansion Properties of Perovskite Materials for Fuel Cell Applications",

- "Pure" and mixed rare earth manganites: HoMnO₃, CaMnO₃, SrMnO₃, Bi_{0.5}Sr_{0.5}MnO₃, Sr_{0.7}Ce_{0.3}MnO₃, Sr_{0.9}Ce_{0.1}MnO₃, Sr_{0.9-x}Ca_xCe_{0.1}MnO₃, Sr_{0.5}Ca_{0.5}MnO₃, Sr_{1-x}Ca_xMnO₃
- Rare earth chromite-based perovskites: $LaCr_{0.75}Mg_{0.25}O_3$, $La_{0.9}Ca_{0.1}CrO_3$, $Sm_{0.9}Sr_{0.1}CrO_3$, $La_{0.9}Gd_{0.1}CrO_3$, $Y_{1-x}Ca_xCrO_3$, $Nd_{1-x}Ca_xCrO_3$, $Sm_{1-x}Ca_xCrO_3$, $Sm_{1-x}Ca_x$
- Mixed rare earth cobaltites and cobaltite-chromites: $Dy_{0.7}Gd_{0.3}CoO_3$, $Tb_{0.8}La_{0.2}CoO_3$, $Nd_{0.4}Eu_{0.6}CoO_3$, $Pr_{0.4}Gd_{0.6}CoO_3$, $Sm_{0.5}Gd_{0.5}CoO_3$; $HoCo_{0.5}Cr_{0.5}O_3$, $DyCo_{0.5}Cr_{0.5}O_3$, $GdCo_{0.5}Cr_{0.5}O_3$
- Mixed aluminates: $Gd_{0.4}Nd_{0.4}AlO_3$, $Nd_{0.8}Tb_{0.2}AlO_3$, $Pr_{0.9}Sr_{0.1}AlO_{3-x}$
- Double perovskites A₂MM'O₆: Sr₂NiMoO₆, Sr₂FeNbO₆, Sr₂GaSbO₆.

Perovskites

Leonid Vasylechko's activities

Thermal Expansion Properties of Perovskite Materials for Fuel Cell Applications

Thermal expansion of CaMnO₃

Chemical name: Calcium Manganese Oxide Chemical formula: CaMnO₃ Crystal structure at RT; *Pnma*, *a* = 5.281 Å, *b* = 7.453 Å, *c* = 5.266 Å Powder Patterns: 00-003-0830, 00-045-1266, 00-050-1746, 00-063-0466, 01-079-6765

CaMnO₃-based ceramics are considered as promising materials for use as cathodes and anodes in SOFC [1, 2] and thermoelectric materials [3-5].

At the ambient conditions, both stoichiometric CaMnO; and oxygen delicient CaMnO3-6 adopt orthorhombic perovskite structure isotypic with GdFeO3 [6, 7 and Refs. herein]. On the heating, orthorhombic CaMnO3-5 undergoes successive phase transitions to the tetragonal structure at 1169 K and than to the cubic perovskite structure at 1186 K. as it was examined by thermal analysis and high-temperature X-ray diffractometry [8]. The same sequence of concentration- and temperature-induced phase transitions (Phnm - 14/mcm - R3c) was further revealed in Ca1-sSr, MnO3-a series by in situ high-temperature neutron diffraction [9]. Structural changes in CaMnO_{3-a} occurred at the heating are accompanied with the oxygen loss [1, 8, 10]. It was reported [10], that orthorhombic CaMnO_{1.6} phase is stable at 973-1023 K when δ <0.04 and the phase transition from the orthorhombic to tetragonal structure occurs in the narrow range 0.02<6<0.04 In Ref. [1] direct change from orthorhombic to the cubic perovskite structure was observed at the temperatures higher than 1073 K, possibly due to the fast loss of oxygen due to the high surface area. No intermediate tetragonal modification was also observed in of CaMn₁,Nb₂O_{5.6} series [4], in which orthorhombic-to-cubic phase transition temperature increases from 1090 K to 1200 K for x=0.02 and x=0.10 samples, respectively. Partial substitution of Mn for tangsten ions in CaMn1xW3O16 series also led to increasing transition temperature from 1171±4 K for the "pure" CaMnO1+5 to 1244±4 K for CaMno 95 W0.05O3 6 [5].

Thermal behaviour of CaMnO₃ perovskite structure has been studied in the temperature range 10 K \leq T \leq 550 K by neutron time-of-flight total scattering [8] and by *in situ* X-ray synchrotron powder diffraction in the temperature range of 10 K - 1073 K [7]. The temperature dependence of the lattice parameters of CaMnO₃ (Fig. 1) is somewhat unusual because the orthorhombic *Phinn* structure becomes metrically tetragonal due to the lattice parameters crossover at two different temperature regions (*ca.* 573 K and 773 K). Lattice parameters of different structural modifications of CaMnO₃-based materials at different temperatures, collected from diverse literature sources are presented in Table 1.





Table 1. Lattice parameters of CaMnO3-based materials at different temperatures

Composition	т, к	S.G., syngony	o, A	h, Å	c.A	Ref
CaMnO;	RT	Pnma	5.274	7.467	5.277	[13]
CaMnO _{3.8}	RT	Pinna	5.281	7,453	5.266	[10]
CaMnO ₁	RT	Pnma	5.3226	7.5103	5.3110	[1]
CaMnO:	RT	Phum	5.2641	5,2782	7.4546	[14]
CaMnO ₂	RT	Phum	5.2659	5:2779	7.4534	[9]
CaMnO:	302	Pnma	5.2816	7.4573	5.2675	[7]
CaMnO _{2.48}	RT	Or	5.282	5.265	7,452	[8]
CaMnO _{2.05}	1173	Tet	5.333	-	7.534	[8]
CaMnO _{2.85}	1193	Cub	3.774	1.11	1.1	[8]
CaMnO:	298	Phan	5,26746	5,28287	7.45790	[11]
CaMnO ₁	1073	Pham	5:31816	5.31251	7.52545	[11]
CaMnO;	10.	Pama	5.2757	7.4398	5.2555	[12]
CaMnO:	130	Pnma	5.2782	7.4435	5,2577	[12]
CaMnO ₃	300	Pnma	5.2816	7.4567	5,2671	[12]
CaMnO ₃	425	Pnma	5.2850	7.4666	5.2748	[12]
CaMnO	550	Pruna	5.2884	7.4761	5,2820	[12]
CaMnOs.a	RT	Pnma	5.2782	7.4529	5.2695	[5]
CaMnous WaasOs	298	Pnma	5,2959	7,4825	5,2964	[5]
CaMno, as Nbau Oa	298	Pnma	5.2884	7.4639	5,2748	[4]
CaMna.osNbra2O1	773	Pnma	5.3125	7.5239	5.3153	[4]
CaMnaoaNbaa2O3	973	Pama	5.3288	7.5463	5.3310	[4]
CaMnaw NbranOa	1073	Pnma	5.3426	7.5595	5,3363	[4]
CaMn _{0.08} Nb _{0.02} Or	1173	Pm3m	3.7901	11	1.41	[4]

Perovskites

Leonid Vasylechko's activities

Dilatometric investigations of CaMnO3 were performed in [1, 3, 10, 15, 16]. Relative linear expansion ($\Delta L/L_0$) of orthorhombic phase increases almost linearly with the temperature, which results in only weak variations of the thermal expansion coefficient (TEC) within 393-873 K (Fig. 2), where oxygen exchange is suppressed [10]. Abnormal maximum of TEC near 1170 K (Fig. 2, right panel) are associated with the phase transition from orthorhombic to the tetragonal phase, which is connected with oxygen loss at further heating. The rise of the thermal expansion coefficient with temperature and oxygen loss above 870 K is related with the formation of Mn37 cations with the size larger than of Mn4+ cation [10]. In the low-temperature range, both thermal expansion and linear TEC (Fig. 2, insets) show clear anomalies, reflecting a secondorder ferromagnetic transition in CaMnO₃ at the Neel temperature $T_N = 124.2$ K, which was determined from the molar heat capacity data [15]. In Ref. [16], the linear thermal expansion coefficient, heat capacity and thermal conductivity of nominally pure and Eusubstituted CaMnO3 were simulated by using molecular dynamics method in the temperature range from 300 K to 700 K. Calculated values of TEC agree well with experimental data (Fig. 2, right panel).





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Hydrogen Storage Materials



Report about the activity of Task group "Hydrogen storage materials" in 2017



Ihor Zavaliy

Physico-Mechanical Institute, National Academy of Sciences of Ukraine

Grant-in-aid № 03-05 "XRD Reference Patterns of Intermetallic Compounds

and Their Hydrides"

25 XRD patterns and the crystal structure data of the intermetallic compounds and their hydrides were submitted to ICDD database. XRD patterns and crystal structure of new $TiZr_3Ni_2N_{0.5}$ subnitride and its hydride, $TiZr_3Ni_2N_{0.5}H_{11}$, are presented as an example below.





Property files for Intermetallic Compounds and Their Hydrides

30 property files of the intermetallic compounds and their hydrides were prepared. Property sheet with capacity decay curves as a main characteristic for MH electrode materials is presented as an example / see file →

List of Property files:

P-c-T diagrams for IMC-H2 systems:

1) Pr_2Ni_7 +H2 2) La_4MgNi_{19} + 3) Pr_4MgNi_{19} 4) Pr_3MgNi_{14} 5) $Nd_2MgCo_9H_x$ 6) $Nd_{2,15}Mg_{0,8}Co_9H_x$

Hydrogen sorption-desorption properties of IMC:

7) $Ho_{1-x}Ti_xCo_2H_x$ 8) $Zr_{1-x}Ti_xCo$ 9) $Mg_{17}Ba_2H_x$ 10) $Ti_{0.9}V_{0.1}/Ti_{0.8}V_{0.2}$ 11) $Zr_6FeAl_2H_x$ 12) $Zr_6NiAl_2H_x$ 13) $Zr_6FeGa_2H_x$ 14) $Ti_4Ni_2N_{0.5}$ 15) $Ti_3ZrNi_2N_{0.5}$

Electrochemical properties of MH electrodes:

16) $Ti_2(Ni,Co)$ 19) $La_{0.5}Nd_{0.5}MgNi_4$ 20) $La_{0.5}Nd_{0.5}MgNi_3Co$ 21) $La_{0.5}Pr_{0.5}MgNi_4$ 22) $La_{0.5}Pr_{0.5}MgNi_3Co$ 23) $PrMgNi_4$ 24) $PrMgNi_3Co$ 25) $Mg_2Co_{0.5}Ni_{0.5}H_x$

and others

Electrochemical hydrogenation properties of Ti₂Ni_{1-x}Co_x alloys

Parent Compound:

Chemical name: Titanium Nickel Cobalt Chemical formula: $Ti_2Ni_{0.5}Co_{0.5}$ Crystal structure: *Fd-3m*, *a*= 11.31(1) Å [1] Powder Pattern: 04-005-4061

Hydride:

Chemical name: Titanium Nickel Cobalt Hydride Chemical formula: Ti₂Ni_{0.5}Co_{0.5}H_{2.73} Crystal structure: *Fd*-3*m*, a= 11.892 Å [2] Powder Pattern: 01-081-4729

Alloys of nominal composition $Ti_2Ni_{1-x}Co_x$ (x=0; 0.02; 0.2; 0.4) were prepared by arcmelting and chill casting in a copper hearth under argon protection and with repeated melting and turning to ensure homogeneity. The alloy ingots were crushed and ground to powders of below 100 mesh using a Fritsch Planetary Mill (Pulverisisette 5). The powder was mixed with 10 wt.%. polyvinyl alcohol (PVA) solution at 10:1 ratio. Charge/discharge cycles were applied by using an in-house automatic unit. The obtained results are shown in Figs. 1 and 2 [3].





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New Ceramics Subcommittee members

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Semiconductor Subfile: M. Delgado and A. Davydov 3/14/2018

Specialty Set 68 (925 entries)

• 20 compounds assigned to SEM:

e.g., Se, Tl₂S, CuBiSe₂

• 6 of which have CER + SEM assignment: e.g., CsInGeS₄



Property database

- Selected ~30 industrially important semiconductor materials
- Compiled physical properties for 15 III-V binary compounds

(led by A. Davydov and G. Komarova)

• 15 Ternary and quaternary compounds have been identified (led by M. Delgado)

15 Binary Compounds from III-V Systems





Galina Komarova Dept. Physics, MSU (Russia)

• Structural data; phase diagrams; electronic, optical and transport properties

(001) GaAs

- Future work:
 - Alloys $In_{1-x}Ga_xN$: lattice parameters vs. x; E_g vs x
 - Metastable phases
 - Low-dimensional materials:
 - epitaxial, strained, 2-dimensional layers
 - Quantum dots



Gallium Nitride GaN

Industrial importance:

optoelectronics (blue-green LEDs), electronics (high-power/high-temp. transistors) Crystal Structure:

Stable: wurtzite P63mc(186); a=3.190(1) Å, c=5.189(1) Å [1] *Metastable:* zinc-blende F-43m (216) a=4.51 Å; rock-salt Fm-3m (225) a=4.006 Å

Physical Properties:

T_{melting} = 2519 °C @ 4.8·10⁴ atm (T_{decomposition} = 779 °C @ 1 atm) [2]

Thermal properties: TCE: $a = 5.59 \cdot 10^{-6} \text{ K}^{-1}$; $c = 3.17 \cdot 10^{-6} \text{ K}^{-1}$ [3]; thermal conductivity

Electronic Properties:

E^{direct} = 3.39 eV (W), 3.2 eV (ZB) @ 300K

Electrical Properties:

Mobility: $\mu_n \leq 1000 \text{ cm}^2 \cdot \text{V} \cdot \text{s}$; $\mu_n \leq 200 \text{ cm}^2 \cdot \text{V} \cdot \text{s}$ Breakdown field: ~ $5 \cdot 10^6 \text{ V} \cdot \text{cm}^{-1}$

Optical Properties:

IR refractive index: n_x=2.3; PL data

1052 K 750 Liquid + GaN GaN+Gas 500 250 Ga + GaN 20 ⁴⁰ at. % N ⁶⁰ 80 100

Fig. 3 Section of the P-T-x diagram at 1 atm pressure of N_2 : peritectic line at 1052 K indicates the upper stability limit of GaN above which GaN decomposes incongruently into liquid (Ga-rich) and gas (N_2)

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Bioceramic Task Group

Dr Charlene Greenwood

Cranfield University, UK.

Bioceramic Definition

A ceramic used as a biomaterial. Biomaterials are substances, synthetic or natural in origin, which can be used as whole or as part of a system to treat, augment, or replace any tissue, organ, or function within the body. These inorganic, solid, crystalline materials must be highly biocompatible and antithrombogenic. They are used in prosthetics, bone implants, implant coatings, joint replacement, dental restoration and tissue engineering, including (but not limited to) the following systems: calcium phosphates (synthetic and natural); calcium sulfates; bioactive glasses and glass ceramics; titanium oxides; alumina; zirconia.

Plan for Bioceramic Task Group

How will I define PDF patterns as a Bioceramic?

- Liaise with Scott Misture, who has previously worked on Bioceramic patterns
- Research into what materials are currently defined as a biomaterial/ bioceramic
- Internet searches, books (e.g. Hench 2003: An Introduction to Bioceramics, Park 2009, Bioceramics: Properties, Characterizations, and Applications), journals (e.g. Bioceramic)
- Natural bioceramics tend to be Calcium Phosphate phases, use this as a starting point then extend the search to synthetic materials

Synthetic Hydroxyapatite

- Producing various synthetic HA with varying amounts of carbonate to mimic biological HA
- Calcium Nitrate Tetrahydrate + Ammonium Phosphate Dibasic = Stoichiometric HA
- Add sodium bicarbonate = Carbonated HA (B-Type)
- Heat stoichiometric HA and B type HA = A-Type and AB-Type HA
- Characterise using XRD and IR

Repeatability of Si-doped and non-doped experimental samples

- Tested Si-doped and non-doped for 0.5 g sample and 0.02 g sample
- Use of internal standard for accuracy in refinement of lattice parameters:
 - NIST SRM 2910a: Calcium Hydroxyapatite
 - Porcine bone
- Some significant differences present between Si-doped values and non-doped values



New members?

- Emily Arnold (PhD Student) : Assist with the characterisation of materials
- Plan to recruit more members to help with subcategories of bioceramics such as glasses, metals, calcium phosphate, by-products etc

Battery Materials Subfile

Update - SpecialtySet68 (925 entries):

- 10 compounds assigned to BAT:
 e.g., LiMn(PO₄); LiCo_{0.8}Mn_{0.1}Ni_{0.1}O₂; Nb₂O₅
 (2016: 26 compounds; 2017: 13 compounds)
- **8** of which are electrode materials for lithium-ion batteries or pseudocapacitors
- 1 of which is an electrode material for potassium-ion batteries
- **1** of which is a electrolyte material for solid-state lithium-ion batteries

Highlights in New Battery Materials: 2017-2018

- 2D transition metal carbides and nitrides (MXenes)
- Metal organic frameworks
- Solid electrolytes for all solid state lithium-ion batteries
- Potassium-ion batteries
- Electrode architectures

2D Transition Metal Carbides and Nitrides



X

Sc,C

Zr.N

V,N

Cr,N

(Ti,V),C

Metal Organic Frameworks

Review

Metal-Organic Frameworks for Energy Applications

Hailong Wang, 1 Qi-Long Zhu, 1 Ruqiang Zou, 2,* and Qiang Xu 1,*



Figure 2. Crystal Structures of Four Representative MOFs (A) MOF-5. (B) HKUST-1. (C) Mg-MOF-74. (D) ZIF-8. C, gray; O, red; and N, blue. The yellow ball represents the porositie

C, gray; O, red; and N, blue. The yellow ball represents the porosities, and the yellow line shows the topology of ZIF-8.

LETTERS

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mature materials

Conductive MOF electrodes for stable supercapacitors with high areal capacitance

Dennis Sheberla¹, John C. Bachman², Joseph S. Elias¹, Cheng-Jun Sun³, Yang Shao-Horn² and Mircea Dincă^{1*}



Figure 1] Structural schematics of N_3 (HITP)₂, a. Molecular structure of N_1 (HITP)₂, b. Relative size of pores, electrolyte E_4N^+ and BF_4^- ions, and acutonitrile solvent molecules shown in a space-filling diagram of idealized N_1 (HITP)₂. Green, lime, blue, grey, brown, and white spheres represent N_1 , F_1 , C_1 , B_1 and H atoms, respectively.



Figure 3 [Performance of Nig(HITP)_electrodes in a symmetrical supercapacitor cell up to 1V, a. Cyclic voltammetry at a scan rate of 10 m /s⁻¹ at increasing cell voltage. A slight deviation of the CV trace around 1 V from rectangular shape is attributed to a redox process described in the text. b. Galvanostic torage and discharge curves at curver distributed 50, 51, 0.2 0 A⁻¹. C. Klyuicki tot showing the imaginary part wress the real part of impedance in the 62kHz-10 mHz range. The inset shows a zoom-in of the high-frequency part (62kHz-1Hz). d. Capacitance retention under repeated cycling at a curver density of 2 Apr ² for 10:000 cycles.

Solid Electrolytes for All-Solid-State Li-Ion Batteries





Fig. 3. Crystal structure of Li₁₀GeP₂S₁₂. (a) Framework structure and lithium ions that participate in ionic conduction; (b) Framework structure of Li₁₀GeP₂S₁₂; (c) Conduction pathways of lithium ions. (Reprinted from ref. [53] with permission from Nature Publishing Group).



Fig. 5. (a) Crystal structure of cubic Li₂La₃/2r₂O₁₂, (b) Coordination polyhedra around the Li1 and Li2 sites; (c) Three-dimensional conducting network of the Li-ion in cubic Li₂La₃/2r₂O₁₂. (Reprinted from ref. [73] with permission from Chemical Society Japan.).

Fig. 1. Schematic illustration of an all-solid-state lithium battery based on Li-ion conduction.



Fig. 2. Ionic conductivity of Li10GeP2S12 phase in comparison with other kinds of electrolytes. (

Potassium-Ion Batteries

ACS APPLIED MATERIALS

Potassium Secondary Batteries

Ali Eftekhari,***,* Zelang Jian,* and Xiulei Ji***





Review www.acsami.org

Figure 1. Lattice structure of (a) Prussian blue, $KFe^{III}Fe^{II}(CN)_{6}$, and (b) layered $LiCoO_2$ and hypothetically layered $KCoO_2$, where in (b) the counterions are shown in purple, oxygen red, and alkali metal blue. The viewing direction for $LiCoO_2$ and $KCoO_2$ is from the crosssection of the layered structure, which is evident in the case of $LiCoO_2$ but almost indistinguishable in the case of $KCoO_2$.



Figure 4. (A) First-cycle galvanostatic potassiation/depotassiation potential profiles at C/10. (B) XRD patterns of electrodes corresponding to marked SOCs in A. (C) Structure diagrams of different K-GICs, side view (up) and top view (down). Reprinted with permission from ref 82. Copyright 2015 American Chemical Society.

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Figure 4. (a) Comparison of the charge/discharge profiles of $K_sFe[Fe(CN)_6]$ and $Na_5Fe[Fe(CN)_6]$ cathode in nonaqueous Na-ion batteries: Reproduced with permission from ref 51. Copyright 2016 Elsevier. (b) Possible intercalation sites in a Fe[Fe(CN)_6] structure; blue, high-spin Fe; green, low-spin Fe; brown, introgen; orange, carbon. Reproduced with permission of ref 54. Copyright 2013 American Chemical Society.



Figure 1. Schematic illustration of the chemical preintercalation synthesis approach, which was used to incorporate K² ions in the interlayer space of bilayered vanadium oxide. Decomposition of the precursor, $\sigma \cdot V_2 O_3$ powder, in aqueous media is carried out in the presence of K² ions. In the sal–gel process, followed by aging, K² ions together with water molecules are trapped between the growing bilayers of vanadium oxide, leading to the formation of the $\delta \cdot K_0 V_2 O_2 nH_2 O$ are presence of K² ions and water molecules in $\delta \cdot K_0 V_2 O_2 nH_2 O$ are hypothetical, and structure refinement needs to be done to establish the presise erystallographic sites of the interlayer species.



Figure 3. Electrochemical characterization of $\delta \cdot K_{a,b} V_s O_s m I_s O$ nanobells. (a) First charge cycle and second discharge/charge cycle curves at a current rate of C/50. (b) Cyding performance at a current rate of C/15. (c) Rate performance at current rates shown in the figure. Electrochemical testing was carried out in the voltage window of 2.0–4.3 V.

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