

<b>Skema til faglig afrapportering</b>
Forsknings- og Innovationsstyrelsen Bredgade 40 1260 København K
Dato:



### Det Frie Forskningsråd

Det Frie Forskningsråd | Kultur og Kommunikation  
 Det Frie Forskningsråd | Natur og Univers  
 Det Frie Forskningsråd | Samfund og Erhverv  
 Det Frie Forskningsråd | Sundhed og Sygdom  
 Det Frie Forskningsråd | Teknologi og Produktion

Vedr. bevilling fra

### 1. Bevillingshaver, projekttitel og virkemiddel

Sagsnr. (fx 09-012345)	
Bevillingshavers navn og stilling og uddannelse	
Arbejdsplads (adresse, telefon og e-mail)	
Privat (adresse, telefon, email)	
Projektets titel	
Virkemiddel	

### 2. Bevillingsperiode

Oprindelig bevillingsperiode	Fra:	Til:
Faktisk bevillingsperiode	Fra:	Til:
Årsagen til eventuelle væsentlige ændringer i bevillingsperioden		

### 3. Øvrige deltagere (der har fået finansieret løn- eller driftsmidler af bevillingen)

Øvrige deltagere (navn, stilling, uddannelse, arbejdsplads, periode beskæftiget/ansat på projektet, køn (M/K))	
Væsentlige ændringer blandt de øvrige deltagere, og i givet fald årsagen hertil	

#### 4. Økonomi

Bevillingens oprindelige størrelse	Ekskl. overhead:	Inkl. overhead:
Eventuelle tillægsbevillinger	Ekskl. overhead:	Inkl. overhead:
Væsentlige afvigelser mellem budget og regnskab og i givet fald årsagen hertil		
Evt. medfinansiering fordelt på arbejdsplads og andre		

Er der indsendt slutregnskab? (sæt X)

Ja

Nej

#### 5. Kvalitativ afrapportering

Vejledning:

I rubrikken nedenfor gives en kort beskrivelse af projektets formål og hovedresultater. Afrapporteringen skal minimum fylde 3.200 anslag og indeholde følgende:

- Hvad var projektets formål, hypoteser, problemstillinger, teorier, metode, data og milepæle?
- Er der væsentlige faglige afvigelser fra projektets oprindelige plan og og i givet fald hvilke?
- Hvad er projektets videnskabelige resultater, og hvordan bidrager disse til opfyldelsen af projektets formål og/eller hypoteseafprøvning?
- Er der fremkommet vigtige spørgsmål og/eller områder for videre forskning?

#### Kvantitativ afrapportering

Vejledning:

Du anbefales at bruge punktopstilling for hver rubrik.

#### 6. Stipendier

Ph.d.-stipendier/grader (navne, arbejdsplads, antal måneder finansieret af bevillingen, køn (M/K))	
Postdocstipendier (navne, arbejdsplads, antal måneder finansieret af bevillingen, køn (M/K))	

## 7. Publikationer affødt af det finansierede projekt

Vejledning:

Oversigten er udarbejdet i overensstemmelse med universiteternes registreringssystem for publikationer og følger samme definitioner af publikationstyper. Kun de publikationstyper, som er væsentligst for Det Frie Forskningsråd, er omfattet. For hver publikationstype skal angives forfatter, titel, sideantal, evt. tidsskrift, og årstal. Desuden skal der for hver publikation angives evt. publicering i Open Access (OA), samt hvor stor andel af publikationen, der skønmæssigt er finansieret af bevillingen i procent (X %).

### Forskning

Artikler, peer reviewed	
Artikler, ikke peer reviewed	
Doktordisputater	
Ph.d.-afhandlinger	
Videnskabelig bøger/antologier	
Videnskabelige rapporter	
Bidrag til bøger/antologier/rapporter	
Working papers/arbejdsrapporter/preprints	
Konferenceartikler, peer reviewed	
Konferenceartikler, ikke peer reviewed	
Patenter	

<b>Datasæt (x hvis afleveret til Dansk Data Arkiv)</b>	
<b>Planlagte publikationer (angiv type)</b>	

#### **Formidling**

<b>Fx forskningsformidlende bøger/antologier, kronikker</b>	
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#### **Rådgivning**

<b>Fx artikler, videnskabelige rapporter</b>	
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#### **Undervisning**

<b>Fx lærebøger, kompendier</b>	
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#### **8. Andre resultater/spin off affødt af projektet**

<b>Nyt samarbejde nationalt og internationalt</b>	
<b>Nye ansøgninger</b>	
<b>Ny finansiering</b>	
<b>Nye teknologier</b>	
<b>Nye produkter</b>	
<b>Nye virksomheder</b>	



**Bilag 1- Participants in Danscatt activities 2010**

<b>Groupleader</b>	<b>VIP's (professors, senior scientists etc.)</b>	<b>Postdocs</b>	<b>Ph.D. students</b>	<b>Students</b>	<b>TAP's (technicians, administrative staff etc.) and scientific assistants</b>
<b>Bo Brummerstedt Iversen,</b> Dept. of Chemistry, Aarhus University	Bo Brummerstedt Iversen Finn Krebs Larsen Henrik Birkedal Jacob Overgaard Jens Erik Jørgensen Torben Rene Jensen Mogens Christensen	Brian R. Pauw Helle Svendsen Henrik Fanø Clausen Jianli Mi Nina Lock Simon Johnsen Stephan Scheins Ye Sun	Casper Ibsen Christoffer Tyrsted David Aarup Dmytro Korablov Dorthe Ravnsbæk Hanna Leemreize Hao Yin Jakob Eltzholtz Kasper Borup Kirsten Ø. Jensen Lasse Bjerg Lene M. Arnbjerg Line Rude Mads Ry Jørgensen Martin Søndergaard Mette Schmøkel Mette Ø. Sjøberg Morten Brix Ley Niels Bindzus Peter Nørby Sebastian Christensen Simone Cenedese Sofie Kastbjerg Thomas Kollin Nielsen Yanbin Shen	Anders B. Blichfeld Anders J. Mørup Casper Clausen Cathrine Holm Olesen Ellen Jensen Espen D. Bøjesen Espen Eikeland Fiona L. Bach-Gansmo Guillermo Gonzalez Henrik Hellstern Jacob Haurum Jagoba Erromo Kevin Henriksen Lars H. Jepsen Lise H. Sørensen Mads K. Hjortshøj Maja L. Jensen Marc E. Kristensen Marie Krogsgaard Martin Schmidt Michael Bay-Andersen Mie Birkbak Mikkel V. Andersen Mogens Schulz Nielsen Payam Javadian	Aref Mamakhel Bo Richter Britta Lundtoft Jacob Becker Jakob Olsen Marianne Sommer Peter Hald

				Per Runge Christensen Peter Thygesen Rudi Stallbohm Simon Froelich Solveig R. Madsen Steffen Pedersen Uffe Filsø Vicki Nue	
<b>Søren Skou Thirup,</b> Dept. of Molecular Biology, Aarhus University	C.B.F. Andersen Ditlev E. Brodersen Gregers Rom Andersen Hanne Poulsen Klaus H. Nielsen Poul Nissen Rune Hartmann Søren Thirup Thomas Boesen	Anne-Marie Winther Bertrand Arnou Chrysa Latrick Claus Olesen Francesca Magnani Henning Tidow J. Jensen Jacob F. Cramer Kai-Tuo Wang Laure Yatime Lee E. Sanderson Linda Schuldt Maike Bublitz Maria Nyblom Mickael Blaise Pontus Gourdon	Adriana K. Kantcheva Andeas Bøggild Anna Dippel Lande Daniel Mattle Dovile Vaicaityte Emil Dedic Helle Kristiansen Ingrid Jurkova Jacob Lauwring Andersen Jesper S. Johansen Jonas L. Gregersen Kaare Bjerregaard- Andersen Kim Langmach Hein Lina Malinauskaite Mette Laursen Michael Jakob Clausen Nick Stub Laursen Nikolaj Drachmann Ole Hamming Oleg Sitsel	A. Allik A. Kotsubei A. Ravichandran Aisha Rafique C. Dellgren H. Alsarraf J.M. Wong P.A. Paulsen T. Sommer T.B. Steffensen	

			Paulina Seweryn Rune T. Kidmose Søren F. Midtgaard Xiangyu Liu Yangzi He Yonathan Sonntag		
<b>Henning Friis Poulsen,</b> Risø DTU, Materials Research Division, Technical University of Denmark	Asger B. Abrahamsen Dorte Juul Jensen Erik Knudsen Erik Mejdal Lauridsen Grethe Winther Henning Friis Poulsen Jean-Claude Grivel Jette Oddershede Martin Meedom Nielsen Niels Bech Christensen Niels Hessel Andersen Poul Norby Søren Schmidt Tejs Vegge Wolfgang Pantleon	Kristoffer Haldrup Ulrik Lund Olsen Yubin Zhang Yue Zhao	Anders Wulff Dadi Sveinbjörnsson Dong He Jacob Larsen Karolina Martyniuk Morten Rask Rasmus Toft-Petersen Stefan Poulsen Tim Brandt van Driel		Peter K. Willendrup
<b>Jens Wenzel Andreasen,</b> Risø DTU, Risø National Laboratory for Sustainable Energy, Technical University of Denmark	Jens Wenzel Andreasen		Arvid Böttiger Jan Kehres Morten Vestager Madsen Thomas Tromholt		
<b>Luise Theil Kuhn,</b> Risø DTU, Fuel Cells and Solid State Chemistry Division	Luise Theil Kuhn	Franz Bræstrup			



<b>Kenny Ståhl</b> , DTU Chemistry, Technical University of Denmark	Kenny Ståhl Pernille Harris		Christian G. Frankær Monica Nøhr Løvgreen	Marianne V. Knudsen	
<b>Tobias Dokkedal Elmøe</b> , DTU Chemical Engineering, Technical University of Denmark	Jan-Dierk Grunwaldt	Matthias Bauer Tobias Dokkedal Elmøe	Alexey Boubnov Jakob Munkholt Christensen Matthias Beier Martin Høj Nikolai Musko		Anders Tiedje
<b>Cathrine Frandsen</b> , DTU Physics, Technical University of Denmark	Cathrine Frandsen Steen Mørup		Erik Brok		
<b>Finn E. Christensen</b> , DTU Space, National Space Institute, Technical University of Denmark	Anders C. Jakobsen Carl B. Jørgensen Finn E. Christensen Irfan Kuvvetli		Nicolai F. Brejnholt		
<b>Robert Feidenhans'l</b> , Niels Bohr Institute, University of Copenhagen	Bente Lebech Brian Møller Andersen Emmanuel Farhi Henning Osholm Sørensen Jens Als-Nielsen Jens Jensen Kim Lefmann Nicolas Bovet Niels Harrit Robert Feidenhans'l Susan Stipp Thomas Bjørnholm	Andrea Prodi Dirk Mueter Kim Dalby Knud Didriksen Kristoffer Haldrup Linda Udby Mark Laver Martin Andersson	Dmitry Khakhulin Ivan Pasarin Jana Baltser Jonas Okkels Birk Karina Sand Kasper Skov Kjær Magni Glyvradal Morten Christensen Simon Oddsson Mariager Tine Straasø Torben Hugaard Jensen Torsten Lauridsen	Alberto Cereser Evgeniy Shkondin Gitte Stieper Henrik Jacobsen Johan Jacobsen Kenneth M. Larsen Lea Hildebrandt Rossander Mads Bertelsen Maria Thomsen Marius Simonsen Mikkel Schou Nielsen	Bente Juhl Andersen Kaspar Klenø Keld Theodor Klas Risveden

			Yun Gu	Morten Sales Pia Jensen Sepide Hakim Sonja Lindahl Holm Stefan Pedersen Ursula Bengård Hansen	
<b>Kell Mortensen,</b> Dept. of Natural Sciences, University of Copenhagen	Jes Knudsen Kell Mortensen Knud J. Jensen Lars Øgøndal Lise Arleth Steen L. Hansen	Jacob Kirkensgaard Jens Bæk Simonsen Rasmus Høiberg- Nielsen	Henrik Munch Jesper Nygaard Leila Malik Nicholas Skar Gislinge Stine Rønholt Søren Kynde Søren Roi-Midgaard		
<b>Michael Gajhede,</b> Dept. of Medical Chemistry, University of Copenhagen	Bente Vestergaard Jette Sandholm Kastrup Karla Frydenvang Katrine Nørgaard Toft Michael Gajhede Ole Kristensen Osman Mirza	Annette Langkilde Charlotte Helgstrand Christian Krintel Heidi Assenfeldt Ernst Helle Hald Taru Deva Wimal Ubhayasekera	Ann-Beth Nørholm Azadeh Shahsavari Christine Ussing Jan Kristensen Jeppe Olsen Johanne Mørch Jensen Lina Juknaite Line Hytloft Kristensen Line Aa. H. Thomsen Magda Møller Malene Hillerup Jensen Monica Fiorentini Paola Sciortino Raminta Venskutonyte Sanjeevani Sooriyaarachchi Thomas Bielefeldt	Amara C. Ditta Björg Eythorsdóttir Bjørn Wisbech Sangill Casper Bennike Fatemeh M. Tabrizi Ingvar Runar Møller Jeppe Olsen Jesper Skov Neergaard Lotte Solvang Christensen Mette Høgh Jensen Thea S. Wind	Heidi Peterson Lise Baadsgaard Sørensen Rico Lehmann

			Steffensen Tina Vognsen Xiaole Wang		
<b>Leila Lo Leggio,</b> Dept. of Chemistry, University of Copenhagen	Anders Kadziola Anders Ø. Madsen Høgni Weihe Jesper Bendix Leila Lo Leggio Marité Cardenas Ole Faurskov Nielsen Sine Larsen Stergios Piligkos	Folmer Fredslund Majbritt Thymark	Anna Åkesson Christian Thuesen Dinna Kruger Ditte Welner Harm Otten Jesper Langholm Jensen Kim K. Rasmussen Magnus Schau- Magnussen Marc Sigrist Maria Wadsäter Pernille Galberg Stig Christoffersen Søs Torpenholt Torben Birk	Erlend Tveten Kasper S. Pedersen Stephanie Ørum Tania Lind Torsten Lauridsen Turi Schäffer Waqas Sethi	Jens-Christian Navarro Poulsen
<b>Alfons Molenbroek,</b> Haldor Topsøe A/S	<b>Permanent staff</b> Alfons M. Molenbroek Anna M. Puig Molina Claus Thomsen Erik O. Törnqvist Fernando Morales Cano Lars Fahl Lundegaard Pablo Beato Robin Christensen Ton V. W. Janssens				

<b>Anette Henriksen,</b> Carlsberg Laboratory, Biostructure Group	Anette Henriksen	Jose Antonio Cuesta Seijo Lyann Sim Michael Skovbo Windahl Rene Jørgensen	Marie Sofie Møller Kristine G. Kirkensgaard		Annette K. Andreassen
<b>Dorthe Posselt,</b> Dept. of Science, Systems and Models, Roskilde University	Bo Jacobsen Dorthe Posselt Kristine Niss Peter Westh	Chunhua Wang	Nicolaj Bagger Thomas Hecksher	Kasper Swiatek	
<b>Beate Klösger,</b> Dept. of Physics and Chemistry, University of Southern Denmark	Beate Klösger		Margaret Hermanowska Olya Krivosheva Raghu Sankar Marsala	Lars Jørgensen Nikoline Vicic- Rasmussen Shen Chen	

## Bilag 2 - List of Publications 2010

### Dept. of Chemistry, Aarhus University

- Becker, J., M. Bremholm, C. Tyrsted, B. Pauw, K.M.O. Jensen, J. Eltzholt, M. Christensen, B.B. Iversen; Experimental setup for in situ X-ray SAXS/WAXS/PDF studies of the formation and growth of nanoparticles in near- and supercritical fluids. *Journal of Applied Crystallography*. **2010**, 43(4), 729-736
- Becker-Christensen, J., L.L. Toft, D.F. Aarup, S.R. Villadsen, M. Glasius, S.B. Iversen, B.B. Iversen; A High Temperature, High Pressure Facility for Controlled Studies of Catalytic Activity under Hydrothermal Conditions. *Energy & Fuels*. **2010**, 2737-2746
- Bianchi, M., D. Guan, S. Bao, J. Mi, B.B. Iversen, P.D.C. King, P. Hofmann; Coexistence of the topological state and a two-dimensional electron gas on the surface of  $\text{Bi}_2\text{Se}_3$ . *Nature Communications*. **2010**, 1(8), 128
- Broomell, C. C., H. Birkedal, C.L. Pinto de Oliveira, J.S. Pedersen, J-A. Gertenbach, M. Young, T. Douglas; Protein cage nanoparticles as secondary building units for the synthesis of 3-dimensional coordination polymers. *Soft Matter*. **2010**, 6, 3167-3171
- Bünger, M.H., H. Oxlund, T.P.K. Hansen, S. Sørensen, B.M. Bibby, J.S. Thomsen, B.L. Langdahl, F. Besenbacher, J.S. Pedersen, H. Birkedal; Strontium and bone nanostructure in normal and ovariectomized rats investigated by scanning small-Angle X-ray scattering. *Calcified Tissue International*. **2010**, 86(4), 294-306
- Bösenberg, U., J.B. Kim, D. Goslar, N. Eigen, T.R. Jensen, J.M. Bellosta von Colbe, Y. Zhou, M. Dahms, D.H. Kim, R. Günther, Y.W. Cho, K.H. Oh, T. Klassen, R. Bohrmann, M. Dornheim; Role of additives in  $\text{LiBH}_4\text{-MgH}_2$  reactive hydride composites for sorption kinetics. *Acta Materialia*. **2010**, 58, 3381-3389
- Bösenberg, U., D.B. Ravnsbæk, H. Hagemann, V. D'Anna, C.B. Minella, C. Pistidda, W. van Beek, T.R. Jensen, R. Bormann, M. Dornheim; Pressure and Temperature Influence on the Desorption Pathway of the  $\text{LiBH}_4\text{-MgH}_2$  Composite System. *Journal of Physical Chemistry Part C: Nanomaterials and Interfaces*. **2010**, 114(35), 15212-15217
- Callini, E., L. Pasquini, L.H. Rude, T.K. Nielsen, T.R. Jensen, E. Bonetti; Hydrogen storage and phase transformations in Mg-Pd Nanoparticles. *Journal of Applied Physics*. **2010**, 108, doi: 10.1063/1.3490206 (7 pages)
- Cerny, R., D.B. Ravnsbæk, G. Severa, Y. Filinchuk, V. d'Anna, H. Hagemann, D. Haase, J. Skibsted, C. Jensen, T.R. Jensen; Structure and Characterization of  $\text{KSc}(\text{BH}_4)_4$ . *Journal of Physical Chemistry Part C: Nanomaterials and Interfaces*. **2010**, 114(45), 19540-19549
- Cerny, R., G. Severa, D.B. Ravnsbæk, Y. Filinchuk, V. D'Anne, H. Hagemann, D. Haase, C.M. Jensen, T.R. Jensen;  $\text{NaSc}(\text{BH}_4)_4$ : A Novel Scandium-Based Borohydride. *Journal of Physical Chemistry Part C: Nanomaterials and Interfaces*. **2010**, 114(2), 1357-1364

- Christensen, A.N., T.R. Jensen, A. Nonat; A new calcium sulfate hemi-hydrate. *Dalton Transactions* (Online). **2010**, 39(8), 2044-2048
- Christensen, M., S. Johnsen, B.B. Iversen; Thermoelectric clathrates of type I. *Dalton Transactions* (Print Edition). **2010**, 39(4), 978-992
- Clausen, H.F., M-A.S. Chevallier, M. Spackman, B.B. Iversen; Three new co-crystals of hydroquinone: crystal structures and Hirshfeld surface analysis of intermolecular interactions. *New Journal of Chemistry*. **2010**, 34, 193-199
- Gauthier, D., A.T. Lindhardt, E.P.K. Olsen, J. Overgaard, T. Skrydstrup; In Situ Generated Bulky Palladium Hydride Complexes as Catalysts for the Efficient Isomerization of Olefins. Selective Transformation of Terminal Alkenes to 2-Alkenes. *Journal of the American Chemical Society*. **2010**, 132(23), 7998-8009
- Gosalawit-Utke, R., J.M. Bellosta von Colbe, M. Dornheim, T.R. Jensen, Y. Cerenius, C.B. Minella, M. Peschke, R. Bormann;  $\text{MgB}_2$  System for Reversible Hydrogen Storage. *Journal of Physical Chemistry Part C: Nanomaterials and Interfaces*. **2010**, 114, 10291-10296
- Herzog, A., M. Marutzky, J. Sichelschmidt, F. Steglich, S. Kimura, S. Johnsen, B.B. Iversen; Strong electron correlations in  $\text{FeSb}_2$ : An optical investigation and comparison with  $\text{RuSb}_2$ . *Physical Review B (Condensed Matter and Materials Physics)*. **2010**, 82(24), 245205
- Ibsen, C.J.S., H. Birkedal; Modification of bone-like apatite nanoparticle size and growth kinetics by alizarin red S. *Nanoscale*. **2010**, 2(11), 2478-2486
- Iversen, B.B.; Fulfilling thermoelectric promises:  $\beta\text{-Zn}_4\text{Sb}_3$  from materials research to power generation. *Journal of Materials Chemistry*. **2010**, 20, 10778-10787
- Jensen, G.V., M. Bremholm, N. Lock, R. Deen, T.R. Jensen, B.B. Iversen, M. Niederberger, J.S. Pedersen, H. Birkedal; Anisotropic Crystal Growth Kinetics of Anatase  $\text{TiO}_2$  Nanoparticles Synthesized in a Nonaqueous Medium. *Chemistry of Materials* **2010**, 22, 6044-6055
- Jensen, T.R., T.K. Nielsen, Y. Filinchuk, J-E. Jørgensen, Y. Cerenius, Yngve, E. MacA. Gray, C.J. Webb; Versatile in situ powder X-ray diffraction cells for solid-gas investigations. *Journal of Applied Crystallography*. **2010**, 43, 1456-1463
- Johnsen, S., M. Christensen, B. Thomsen, G.K.H. Madsen, B.B. Iversen; Barium dynamics in noble-metal clathrates. *Physical Review B (Condensed Matter and Materials Physics)*. **2010**, 82(18), 184303
- Jørgensen, M.R.V., H.F. Clausen, M. Christensen, R.D. Poulsen, J. Overgaard, B.B. Iversen; Crystal Structures and Physical Properties of Three New Manganese-Based

Coordination Polymers with p-Biphenyldicarboxylic Acid Linkers. *European Journal of Inorganic Chemistry*. **2010**, 2011(4), 549-555

Jørgensen, J-E., T.C. Hansen; High-pressure neutron diffraction study of BaFe<sub>2</sub>As<sub>2</sub>. *European Physical Journal B. Condensed Matter and Complex Systems*. **2010**, 78(4), 411-415

Jørgensen, J-E., J.S. Olsen, L.I. Gerward; Compression mechanism of GaF<sub>3</sub> and FeF<sub>3</sub>: a high-pressure X-ray diffraction study. *High Pressure Research*. **2010**, 30(4), 634-642

Laumann, A., K.T. Fehr, M. Wachsmann, M. Holzapfel, B.B. Iversen; Metastable formation of low temperature cubic Li<sub>2</sub>TiO<sub>3</sub> under hydrothermal conditions — Its stability and structural properties. *Solid State Ionics*. **2010**, 181, 1525-1529

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Lock, N., Y. Wu, M. Christensen, L.J. Cameron, V.K. Peterson, A.J. Bridgeman, C.J. Kepert, B.B. Iversen; Elucidating Negative Thermal Expansion in MOF-5. *Journal of Physical Chemistry Part C: Nanomaterials and Interfaces*. **2010**, 114(39), 16181-16186

Mi, J-L., M. Christensen, E. Nishibori, V. Kuznetsov, D.M. Rowe, B.B. Iversen; Multitemperature synchrotron powder diffraction and thermoelectric properties of the skutterudite La<sub>0.1</sub>Co<sub>4</sub>Sb<sub>12</sub>. *Journal of Applied Physics*. **2010**, 107(11), 113507

Mi, J-L., M. Christensen, C. Tyrsted, K.O. Jensen, J. Becker, P. Hald, B.B. Iversen; Formation and Growth of Bi<sub>2</sub>Te<sub>3</sub> in Biomolecule-Assisted Near-Critical Water: In Situ Synchrotron Radiation Study. *Journal of Physical Chemistry Part C: Nanomaterials and Interfaces*. **2010**, 114(28), 12133-12138

Mi, J., N. Lock, T. Sun, M. Christensen, M. Søndergaard, P. Hald, H.H. Hng, J. Ma, B.B. Iversen; Biomolecule-Assisted Hydrothermal Synthesis and Self-Assembly of Bi<sub>2</sub>Te<sub>3</sub> Nanostring-Cluster Hierarchical Structure. *A C S Nano*. **2010**, 4(5), 2523–2530

Nielsen, T.K., U. Bösenberg, R. Gosalawit, M. Dornheim, Y. Cerenius, F. Besenbacher, T.R. Jensen; A Reversible Nanoconfined Chemical Reaction. *A C S Nano*. **2010**, 4(7), 3903

Overgaard, J., B.B. Iversen; Charge Density Methods in Hydrogen Bond Studies. *Structure and Bonding*. **2010**, 1-22

Pedersen, B.L., H. Yin, H. Birkedal, M. Nygren, B.B. Iversen; Cd Substitution in M<sub>x</sub>Zn<sub>4-x</sub>Sb<sub>3</sub>: Effect on Thermal Stability, Crystal Structure, Phase Transitions, and Thermoelectric Performance. *Chemistry of Materials*. **2010**, 22, 2375-2383

Pistidda, C., S. Garroni, F. Dolci, E.G. Bardaji, A. Khandelwal, P. Nolis, M. Dornheim, R. Gosalawit, T.R. Jensen, Y. Cerenius, S. Surinach, M.D. Baro, W. Lohstroh, M. Fichtner; Synthesis of amorphous Mg(BH<sub>4</sub>)<sub>2</sub> from MgB<sub>2</sub> and H<sub>2</sub> at room temperature. *Journal of Alloys and Compounds*. **2010**, 508, 212-215

- Platts, J.A., J. Overgaard, C. Jones, B.B. Iversen, A. Stasch; First Experimental Characterization of a Non-nuclear Attractor in a Dimeric Magnesium(I) Compound. *Journal of Physical Chemistry Part A: Molecules, Spectroscopy, Kinetics, Environment and General Theory*. **2010**, 115, 194-200
- Polanski, M., T.K. Nielsen, Y. Cerenius, J. Bystrzycki, T.R. Jensen; Synthesis and decomposition mechanisms of  $Mg_2FeH_6$  studied by in-situ synchrotron X-ray diffraction and high-pressure DSC. *International Journal of Hydrogen Energy*. **2010**, 35, 3578-3582
- Ravnsbæk, D.B., Y. Filinchuk, R. Cerny, M.B. Ley, D. Haase, H.J. Jakobsen, J. Skibsted, T.R. Jensen; Thermal Polymorphism and Decomposition of  $Y(BH_4)_3$ . *Inorganic Chemistry*. **2010**, 49, 3801-3809
- Ravnsbæk, D.B., C. Frommen, D. Reed, Y. Filinchuk, M. Sørby, B. Hauback, H.J. Jakobsen, D. Book, F. Besenbacher, J. Skibsted, T.R. Jensen; Structural studies of lithium zinc borohydride by neutron powder diffraction, Raman and NMR Spectroscopy. *Journal of Alloys and Compounds*. **2010**, doi:10.1016/j.jallcom.2010.11.008 - in press
- Ravnsbæk, D.B., T.R. Jensen; Tuning hydrogen storage properties and reactivity: Investigation of the  $LiBH_4$ - $NaAlH_4$  system. *Journal of Physics and Chemistry of Solids*. **2010**, 71, 1144-1149
- Ravnsbæk, D.B., L. Sørensen, Y. Filinchuk, D. Reed, D. Book, H.J. Jakobsen, F. Besenbacher, J. Skibsted, T.R. Jensen; Mixed-Anion and Mixed-Cation Borohydride  $KZn(BH_4)Cl_2$ : Synthesis, Structure and Thermal Decomposition. *European Journal of Inorganic Chemistry*. **2010**, 2010(11), 1608-1612
- Renzi, P., J. Overgaard, M. Bella; Multicomponent asymmetric reactions mediated by proline lithium salt. *Organic and Biomolecular Chemistry*. **2010**, 8, 980-983
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