

## Impact case study (REF3)

<b>Institution:</b> University of Oxford		
<b>Unit of Assessment:</b> 8 – Chemistry		
<b>Title of case study:</b> SCG-Oxford Centre of Excellence in Chemistry: New functional materials with economic impact		
<b>Period when the underpinning research was undertaken:</b> 2012 - 2019		
<b>Details of staff conducting the underpinning research from the submitting unit:</b>		
<b>Name(s):</b>	<b>Role(s) (e.g. job title):</b>	<b>Period(s) employed by submitting HEI:</b>
Professor Dermot O'Hare	Professor of Organometallic and Materials Chemistry; Director SCG-Oxford Centre of Excellence	01/03/1998 to present
Professor Edman Tsang	Professor of Inorganic Chemistry	01/09/2007 to present
Dr Jean-Charles Buffet	Deputy-Director SCG-Oxford Centre of Excellence (CoE)	02/06/2011 to present
Dr Chunping Chen	CoE Programme Manager	12/06/2013 to present
Dr Dana-Georgiana Crivoi	}	05/09/2016 to 15/07/2019
Dr Jingfang Yu	}	11/05/2016 to present
Dr Yue Wu	}	13/01/2014 to 12/07/2016
Dr Qiang Wang	} Postdoctoral Research	16/06/2011 to 31/08/2012
Dr Hongri Suo	} Assistants working in SCG-	16/11/2015 to 30/09/2018
Dr Alexander Kilpatrick	} Oxford CoE	09/02/2015 to 31/08/2018
Dr Haohong Duan	}	05/01/2015 to 19/10/2018
Dr K. Ruengkajorn	}	01/10/2014 to 11/12/2017
Dr Meng-Jung Li	}	21/01/2013 to present
<b>Period when the claimed impact occurred:</b> 1 <sup>st</sup> August 2013 – 31 <sup>st</sup> December 2020		
<b>Is this case study continued from a case study submitted in 2014?</b> No		
<b>1. Summary of the impact</b> (indicative maximum 100 words)		
<p>Established in 2012, the SCG-Oxford Centre of Excellence for Chemistry (CoE) is a unique collaboration between SCG (a leading business conglomerate in the Association of Southeast Asian Nations (ASEAN)) and Oxford's Department of Chemistry. The CoE focuses on research and development in the fields of advanced materials and catalysis. Its objective is to act as a hub for academic/industry collaboration to drive innovation to SCG and impact for Oxford research. Ground-breaking discoveries have been made: from new catalysts for CO<sub>2</sub> conversion, alkane chemistry, nanomaterials as functional additives in polymer packaging and energy devices. <b>[Text removed for publication]</b> To date three commercial functional materials products deriving from CoE research, <i>CIERRA<sup>TM</sup> Flame Retardant</i>, <i>CIERRA<sup>TM</sup> CO<sub>2</sub> Capture</i> and <i>CIERRA<sup>TM</sup> Barrier</i>, have been launched by SCG Chemicals. In addition to influencing SCG's strategic commercial developments as an R&amp;D led company, the CoE is enhancing UK-Thai relations through skills training, mentoring and inward investment to the UK.</p>		
<b>2. Underpinning research</b> (indicative maximum 500 words)		
<p>In 2012, SCG funded a Postdoctoral Research Fellowship in Oxford's Department of Chemistry to develop new 2D inorganic materials that would be compatible with non-polar polyolefins in order to make new higher value/performance inorganic-polyolefin nanocomposites. This funded research resulted in the discovery of a simple, scalable and cost-effective platform for the synthesis of a stable and transparent dispersion of layered double hydroxides in non-polar hydrocarbons <b>[R1]</b>. This breakthrough enabled the transformation of conventional hydrophobic, mineral-like inorganic material into a dispersible, organophilic platelet system and is the basis of SCG's first inorganic materials additive for PVC. Since 2012 SCG has continued to make substantial R&amp;D investment in order to expand and develop the Oxford developed novel materials platform, trademarked as <i>CIERRA<sup>TM</sup></i>. In a collaborative project, researchers both at the CoE and at SCG R&amp;D have reported that <i>CIERRA<sup>TM</sup></i> is an excellent solid support material for single-site, metallocene polyolefin catalysts <b>[R2]</b>. Commercial metallocene catalysts supported on <i>CIERRA<sup>TM</sup></i> are now in pilot plant trials for the production of high value polyethylene grades.</p>		

In a development of the platform, researchers at the CoE developed reproducible, robust, and scalable syntheses of core-shell hybrid materials containing a microporous zeolite (or a silica) core with an aqueous miscible organic-layered double hydroxide (AMO-LDH) shell using a simple *in-situ* coprecipitation method. These materials now offer new commercial opportunities for SCG in gas adsorption, catalysis and water treatment [R3].

CoE's fundamental research on CO<sub>2</sub> chemistry is supporting SCG's commitment to making a 20% reduction in its CO<sub>2</sub> emissions. As part of this effort, the CoE reported in 2018 the synthesis of ultrathin (1–3 cationic-layers) (CuZn)<sub>1-x</sub>Ga<sub>x</sub>-CO<sub>3</sub> *CIERRA*<sup>TM</sup> nanosheets as a precursor to a solid catalyst for the selective hydrogenation of CO<sub>2</sub> to methanol. This CoE study (O'Hare, Tsang) reported methanol productivity with a space-time yield which, at the time of publication, was higher than all reported Cu-based catalysts in the open literature [R4]. The potential commercial impact and route to market of this catalyst is currently under review by SCG. To support these studies the CoE has performed comparative benchmarking studies with the Clariant and JM commercial catalyst offerings.

The Oxford platform has enabled the CoE to address major challenges in topics related to the Circular Economy. One focus is a 5-year project to create novel approaches for future generation polymer materials for food packaging. Packaging is the largest net contributor to plastic waste in the environment, utilising 40% of global olefin production (source: CS3 white paper on *Science to Enable Sustainable Plastics*, 2020). The CoE has made significant technical breakthroughs in this field by developing a novel approach to making high aspect ratio 2D non-toxic *CIERRA*<sup>TM</sup> nanosheet dispersions. These novel coatings on polymer packaging film will simplify the packing systems, reduce the number of different polymer layers and replace the need for the aluminium barrier layer. The high O<sub>2</sub> and water vapour barrier coating films exhibit an oxygen transmission rate (OTR) for 12 µm PET coated film to below the instrument detection limit (<0.005 cc m<sup>-2</sup> day<sup>-1</sup>) and 60 times better than aluminium coated PET [R5]. Most importantly, these coated films are also transparent and mechanically robust, making them suitable for flexible food packing while also offering new recycling opportunities.

In a further development of the Oxford platform, researchers at the CoE investigated biomass conversion and valorisation. They have reported two breakthrough discoveries related to catalytic hydrodeoxygenation of bio-oil and related substrates. Most recently, PIs in the CoE (O'Hare, Tsang) in collaboration with colleagues at Chinese Academy of Sciences, Beijing, reported that N<sub>2</sub> could be used to reduce the activation energy for catalytic hydrodeoxygenation over ruthenium-based catalysts. Specifically, a 4.3-fold activity increase was reported in the catalytic hydrodeoxygenation of *p*-cresol to toluene over a titanium oxide supported ruthenium catalyst (Ru/TiO<sub>2</sub>) by simply introducing 6 bar N<sub>2</sub> under batch conditions at 160 °C and 1 bar hydrogen. The CoE further demonstrated that N<sub>2</sub> promotion of hydrodeoxygenation can be regarded as a general strategy [R6].

### 3. References to the research (indicative maximum of six references)

All references are journal articles:

[R1] Preparation of stable dispersions of layered double hydroxides (LDHs) in nonpolar hydrocarbons: new routes to polyolefin/LDH nanocomposites; Q. Wang, X. Zhang, J. Zhu, Z. Guo and D. O'Hare, *Chem. Commun.* **2012**, *48*, 7450-7452. DOI: 10.1039/C2CC32708B

[R2] Metallocene supported core@LDH catalysts for slurry phase ethylene polymerisation; J.-C. Buffet, C. F. H. Byles, R. Felton, C. Chen and D. O'Hare, *Chem. Commun.* **2016**, *52*, 4076-4079. DOI: 10.1039/C6CC00280C

[R3] Core-shell zeolite@aqueous miscible organic-layered double hydroxides; C. Chen, C.F.H. Byles, J.-C. Buffet, N. H. Rees, Y. Wu and D. O'Hare, *Chem. Sci.* **2016**, *7*, 1457-1461. DOI: 10.1039/C5SC03208C

[R4] CO<sub>2</sub> hydrogenation to methanol over catalysts derived from single cationic layer CuZnGa LDH precursors; M. M.-J. Li, C. Chen, T. Ayvali, H. Suo, J. Zheng, I. F. Teixeira, L. Ye, H. Zou, D. O'Hare and S. C. E. Tsang, *ACS Catal.* **2018**, *8*, 4390-4401. DOI: 10.1021/acscatal.8b00474

[R5] High oxygen barrier coating using non-toxic nanosheet dispersions for flexible food packaging film; J. Yu, K. Ruengkajorn, D.-G. Crivoi, C. Chen, J.-C. Buffet, D. O'Hare, *Nat. Commun.* **2019**, *10*, 2398. DOI: 10.1038/s41467-019-10362-2

[R6] Hydrodeoxygenation of water-insoluble bio-oil to alkanes using highly dispersed Pd-Mo catalyst; H. Duan, J. Dong, X. Gu, Y.-K. Peng, W. Chen, T. Issariyakul, W. K. Myers, M.-J. Li, N. Yi, A. F. R. Kilpatrick, Y. Wang, X. Zheng, S. Ji, Q. Wang, J. Feng, D. Chen, Y. Li, J.-C. Buffet, S.C.E. Tsang and D. O'Hare, *Nat. Commun.* **2017**, *8*, 591. DOI: 10.1038/s41467-017-00596-3

#### 4. Details of the impact (indicative maximum 750 words)

The CoE's impacts include [text removed for publication] the creation of new breakthrough materials platform technology, assisting in the product development pipeline, and the enhancement of Thai-UK relations through skills training, mentoring and inward investment to the UK.

##### Pathway to impact

SCG is the third largest public company in Thailand and in 2019 was ranked in the top 650 largest public companies in the world by Forbes (sales: USD14,800,000,000, May 2019); it is a leading conglomerate in the ASEAN region with 3 core businesses: SCG Cement-Building Materials, SCG Chemicals and SCG Packaging [E11]. The partnership between SCG and Oxford Chemistry began in 2011, after Professor O'Hare described the new Oxford platform to SCG Chemicals, who agreed to fund three proof-of-concept research projects. Building on the successful outcome of these projects, in 2012 the SCG Board approved the creation of a Centre of Excellence in Chemistry (CoE) to enable development of the Oxford discoveries and provide a stable, long term visionary engagement with Oxford Chemistry. The mission of the CoE is to assist SCG in becoming less reliant on non-proprietary technologies and move into higher value products, whilst forging more synergic links with industry. This allows both parties to advance their mutual long-term objectives of better enabling sustainable development. O'Hare spent a sabbatical year at SCG Chemicals at their headquarters in Bangkok in 2014-15 supported by an EPSRC Impact Acceleration Account (IAA) grant. This further cemented a deeper relationship, mutual respect, trust and appreciation of how Oxford and SCG can effectively work together to deliver lasting impact.

The SCG-Oxford CoE was awarded the 2019 Royal Society of Chemistry Industry-Academia Collaboration Award for creating a unique and long-standing collaboration bringing benefits to chemical science [E1]. The success of the CoE has led to renewal of the Framework Cooperation Agreement, signed in May 2019, extending the collaboration between SCG and the University of Oxford until 2025 [E3].

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##### Enhancing UK-Thai relations

The success of the CoE in building on the CIERRA™ platform, has played a role in enhancing UK-Thai relations. In 2016 Professor O'Hare and SCG were honoured by an audience with HRH Princess Sirindhorn on the occasion of celebrating Thailand-UK Science and Innovation Partnerships – the first time a commercial Thai organisation has been invited to showcase new chemical technologies to the Thai Royal Family [E4]. Thailand's Ambassador to the United Kingdom confirms the benefit of on SCG's relationship with Oxford Chemistry:

*"The SCG-Oxford Centre of Excellence for Chemistry collaboration demonstrates SCG's far-sighted vision to access the scientific and technological developments in the UK with a view to innovating new discoveries for sustainable benefits to humankind. Indeed, this is a perfect project as it relies on the internationally leading research carried out in the CoE and, as a result, SCG has created new materials that are environmentally friendly and can transform our lives in many ways. SCG has become a role model for other Thai businesses in search of excellence and innovations with internationally renowned institutions, like the University of Oxford... Such collaboration also fits in well with Thailand's foreign policy in strengthening of the cordial ties between Thailand and the UK at all levels, and this will benefit not only our two countries, as the international community will stand to benefit from practical and commercially viable innovations from the CoE.*

*This achievement was recognised in 2016 when the Director of the CoE, Professor Dermot O'Hare and SCG's then President... were presented to HRH Princess Maha Chakri Sirindhorn at the British Embassy in Bangkok. This was a tremendous honour for all concerned and the first time a*

*commercial Thai organisation has been invited to showcase new chemical technologies to the Thai Royal Family and was a demonstration of how the SCG-Oxford University collaboration strengthened scientific and commercial ties between the UK and Thailand.” [E4]*

### **CoE research commercialisation and breakthrough technologies at SCG**

Through their support of the CoE, SCG currently has a portfolio of 50 PCT international patent applications describing novel and inventive functional materials technology [E5]. SCG has registered *CIERRA™* (Cierra.com) as their brand name for the new layered double hydroxide functional materials platform technology that was first created at the CoE. SCG state on their website, ‘*SCG has launched the CIERRA™ line of inorganic performance materials to complement our existing high value-added polymer products (HVA). SCG’s technology has been developed in collaboration with Oxford University to control the physical and chemical properties of CIERRA™ to support each application area.*’ [E6]. To date, 3 commercial products have been launched by SCG Chemicals [E7]:

- ***CIERRA™ Flame Retardant*** – At the 12<sup>th</sup> International Wire & Cable Trade Fair for Southeast Asia in 2017, SCG announced *Flame Retardant*, a low smoke, halogen free flame retardant additive that meet quality standards of both domestic and international levels. It requires 4 times lower dosage compared to existing inorganic flame retardant additives, with the added benefit of longer time to ignition, 2 times smoke suppression, and improved char formation.
- ***CIERRA™ CO<sub>2</sub> Capture*** – At FEICA (the most important Conference & EXPO for the adhesive and sealant industry in Europe) in September 2019, SCG announced *CO<sub>2</sub> capture*. *CO<sub>2</sub> Capture* reduces bubbles that are generated during the curing of polyurethane adhesives. This reduction in bubbles results in an adhesion performance increase. In addition to high CO<sub>2</sub> capture, it will help reduce electrical conductivity – a source of potential corrosion issues. *CO<sub>2</sub> Capture* is recommended to be used in polyurethane adhesive formulation in applications such as automotive & rail glazing adhesives, semi-structural adhesives, and PUR hot-melts used for instance in technical textiles.
- ***CIERRA™ Barrier*** – At KFair Dusseldorf (the world’s largest trade fair for plastic and rubber) in October 2019, SCG introduced a mono-material film solution which creates recyclable and transparent food packaging that is able to prevent moisture and O<sub>2</sub> from permeating, and can replace conventional, non-recyclable metallised film. This new mono-material packaging solution contains *CIERRA™ Barrier* a non-toxic, inorganic nanosheets developed by SCG-Oxford CoE.

### **[Text removed for publication]**

The CoE / *CIERRA™* platform has enhanced SCG’s R&D capabilities by facilitating people exchange, with 8 PDRAs and 4 DPhil students from CoE having visited the SCG R&D labs in Rayong, Thailand to carry out large scale pilot testing, technology transfer and SCG researcher training. SCG have sent two Senior Researchers to Oxford for 3-6 month secondments to support the technology transfer from Oxford.

Additional impact directly arising from the close collaboration between SCG and Oxford was realised in a press statement on 12 October 2020 [E10] in which the Thai Ministry of Public Health, Siam Bioscience, SCG and AstraZeneca signed a Letter of Intent on the manufacture and supply of 26,000,000 doses of the University of Oxford’s COVID-19 vaccine AZD1222. **[Text removed for publication]** [E9].

### **5. Sources to corroborate the impact** (indicative maximum of 10 references)

[E1] Website: SCG-Oxford CoE win 2019 Royal Society of Chemistry Industry-Academia Collaboration Award for collaboration bringing benefits to chemical science

[E2] Company Registration of SENFI-UK on Companies House (8 Nov 2017) corroborating SCG’s foreign direct investment in the UK

[E3] *CIERRA™* Press release: SCG opening Begbroke laboratory, Oxford on 02/06/2019 corroborating SCG’s direct investment in the UK and impact on strategic business development

[E4] Thai Embassy letter of support confirming strengthened scientific and commercial ties (Jan 2021)

- [E5] Patents: List of 50 PCT International patent applications arising from the SCG-Oxford CoE describing novel and inventive functional materials technology
- [E6] SCG website: Details of *CIERRA™* products showing Oxford Chemistry collaboration
- [E7] *CIERRA™* website: Details of *CIERRA™ Flame Retardant*, *CO<sub>2</sub> Capture* and *Barrier* showing commercialisation of break-through CoE technologies
- [E8] Engineers Project Profile: Development of SENFI-UK laboratories at Begbroke Science Park showing SCG's direct investment in the UK and impact on strategic business development
- [E9] SCG letter of support confirming Oxford Chemistry collaboration and impacts (Jan 2021)
- [E10] Press release: British Embassy announce partnership between Thailand's Ministry of Public Health, Siam BioScience, SCG and AstraZeneca to manufacture and supply the University of Oxford's COVID-19 vaccine (12 Oct 2020)
- [E11] SCG 2019 Annual Report (page 1) to corroborate SCG's core business structure and R&D programme