Institution: University of Exeter		
Unit of Assessment: UoA 9 Physics		
Title of case study: ARTEMIS: Innovation through advanced modelling of material interfaces.		
Period when the underpinning research was undertaken: 2014 - 2020		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Steven Hepplestone	Senior Lecturer	2014 – Present
Period when the claimed impact occurred: 2015-2020		
Is this case study continued from a case study submitted in 2014? N		

1. Summary of the impact (indicative maximum 100 words)

ARTEMIS is a unique theoretical framework and simulation tool developed at the University of Exeter to explore material interfaces at the atomic scale. ARTEMIS has been **adopted by research-intensive SMEs** in aspects of next-generation energy systems and storage, to focus their R&D activities, **stimulating growth by attracting additional investment** and **accelerating product development.** This has helped to strengthen the UK's technology base in areas such as energy storage and battery technology and has generated over £6.6M in savings and additional investment. For example, Deregallera, an SME based in South Wales, has used ARTEMIS to identify the most promising areas for development, helping it to secure additional investment of at least £4M, make cost savings of £2M and establishing itself as a key partner in the UK's Faraday Battery Challenge.

2. Underpinning research (indicative maximum 500 words)

Interfaces, where two different materials meet, exist in practically all devices. These interfaces often determine the behaviour and efficiency of the device itself. They can, for example, affect how electrical or thermal current flows, or how a battery stores energy.

Born out of condensed matter research at the University of Exeter, we have developed an atomic scale interface modelling package, ARTEMIS **[3.1]**. ARTEMIS is an interface builder which enables the user to predict the most likely structure and properties of an interface between materials. It does this by examining thousands of likely interface structures, characterising them using an energy landscape package (such as DFT) and then evaluating which is "best" according to chosen criteria. ARTEMIS is designed to be almost entirely automated, allowing users with limited computational physics expertise to predict and optimise complex surface structures. It is also the first unified approach to interface prediction and optimisation, incorporating several unique features. For example, it considers all possible terminations of a surface and lattice matching to provide the most likely unit cell structure at the interface between materials. It can also take into account intermixing, allowing analysis of complex, non-uniform interfaces. Finally, it can make a series of predictions regarding the likely physical properties of an interface, and even optimise structures guided by these.

ARTEMIS is designed to interact with several other atomic scale calculation approaches, such as first principle techniques, so that the range of physical properties that ARTEMIS is able to predict is vast. These include: modelling of atomic interfaces in electronic devices **[3.2]**, identifying new phases which form at the interface **[3.2; 3.3]**, predicting heat flow through atomic interfaces **[3.4]**, understanding reaction pathways in batteries **[3.5]** and understanding atomically thin or two-dimensional materials **[3.6]**.

The ARTEMIS theoretical framework was first implemented as a software package in 2016. It was initially used to explore the interface between silicon and barium titanate where there is a reaction which leads to the formation of the Fresnoite phase **[3.3]**. Since then it has been used and extended collaboratively with various companies, mainly SMEs developing devices, to tackle some challenging technical issues. Whilst the majority of the work is covered by NDAs, the core principles are highlighted by the following examples:

(i) Capacitive Energy Storage: In collaboration with Deregallera, exploring the development of capacitor-based devices for energy storage, the capabilities of ARTEMIS were expanded to examine the colossal permittivity materials being used. These materials contain many internal interfaces (called grain boundaries); ARTEMIS helped to explain the observed phenomena **[3.4]**.

(ii) Batteries: Batteries often consist of layered materials. In addition, surface effects are a significant factor in capacity. A key issue in the development of improved battery storage is the interface problems arising from the movement of ions between the layers or onto the surface during operation. Using ARTEMIS, we have been exploring the potential properties of Sn_3N_4 surfaces **[3.5]** and 2D materials **[3.6]**, providing preliminary data to Deregallera and to other companies for new potential battery technologies.

(iii) Solar Cells: ARTEMIS was also developed to model solar cells, and explore how the interface between the active layer and the electrical contacts (via the Schottky barrier effect) can influence the efficiency of the device (this included collaboration with Solaris on the devices it was developing).

(iv) Memory devices and thermoelectric devices: ARTEMIS has also been applied to model novel devices based on silicon oxide interfaces.

These developments have culminated (in 2019) in an academic release **[3.1]** of the ARTEMIS software package (http://www.artemis-materials.co.uk/), making it freely available to academic and industrial researchers.

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

[3.1] Taylor NT, Davies FH, Rudkin IEM, Price C, Chan E, **Hepplestone SP**, *"ARTEMIS: Ab initio Restructuring Tool Enabling the Modelling of Interface Structures,"* Computer Physics, volume 257, pages 107515-107515. (2020) DOI:10.1016/j.cpc.2020.107515

[3.2] Taylor NT, Davies FH, Davies S, Price CJ, **Hepplestone SP**, *"The fundamental mechanism behind colossal permittivity in oxides,"* Adv. Materials.1904746. (2019) DOI: 10.1002/adma.201904746

[3.3] Taylor NT, Davies FH, **Hepplestone SP**. *"First principles electronic and elastic properties of fresnoite Ba2TiSi2O8,"* Materials Research Express 4(12). (2017) DOI: DOI: 10.1088/2053-1591/aa99e8/meta

[3.4] Hepplestone SP and Srivastava GP. *"Theory of interface scattering of phonons in superlattices,"* Phys. Rev. B, **82**, 144303. (2010) DOI: 10.1103/PhysRevB.82.144303

[3.5] Fitch S, Cibin G, **Hepplestone SP**, Garcia-Araez N, & Hector A L. *"Solvothermal synthesis of Sn_3N_4 as a high capacity sodium-ion anode: theoretical and experimental study of its storage mechanism"*. Journal of Materials Chemistry A. (2020) DOI: 10.1039/D0TA04034G

[3.6] De Sanctis A, Amit I, **Hepplestone SP**, Craciun MF, Russo S. *"Strain-engineered inverse charge-funnelling in layered semiconductors,"* Nature Communications 9(1). (2018) DOI: 10.1038/s41467-018-04099-7

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

Research intensive SMEs are key to regional and national economic development. The transformative nature of the high technology products being developed by these SMEs affords significant potential for economic growth particularly in key areas identified by the UK government such as clean growth, energy storage and battery technologies. Over the last five years ARTEMIS has been successfully established as a powerful predictive tool that has helped SMEs (key partner Deregallera and others including Solaris Photonics, Lambda Energy, Anaphite) strengthen the UK's technology base in these important areas.

Adoption of ARTEMIS by Deragallera: Deregallera is an SME developing materials for energy storage and conversion, including a hybrid energy storage system to extend the life of an electric vehicle battery by 50%. The company is a key partner in the UK's Faraday Battery Challenge, a £274M government investment into battery technology through the Industrial Strategy. In 2016 the company began the development of capacitors for energy storage. ARTEMIS modelling allowed them to improve the manufacturing process to maximise the performance of their prototypes (by avoiding the production of a Fresnoite phase at the interface **[3.3]**). This information allowed the company to *"boost their funding to £3M"* **[5.1]** through MOD investment.

Accelerating product development: Subsequent collaborative projects with Deragallera in 2017 and 2018 modelled the interfaces of the CCTO polycrystalline material, to explore further their application in capacitors for energy storage. ARTEMIS modelling helped the company to identify the limitations at an early stage **[3.4]** and to focus instead on battery technology with *"the net saving to the business we estimate to be of the order of £2M."* **[5.2].**

ARTEMIS's predictions for capacitive energy storage led Deragallera to a new area of energy storage using batteries, and has been used to simulate novel battery designs **[3.5]**. The head of Deragallera's materials department, Dr. Peter Curran stated **[5.3]** "*[Dr Hepplestone's] study of Na interactions with nanoparticle surfaces (creating an interface)…helped define the technical barriers to commercial realisation of our battery material. This directly led to…an Innovate UK Award of £958K.*" In addition, predictions from ARTEMIS also suggested a further novel Na battery design based on 2D materials [6] which *"provided us with preliminary data for a new battery design, which was the subject of an Innovate UK award of £437K (IUK App#28977)"* **[5.3]**.

Other divisions within Deregallera are also utilising ARTEMIS to support their technology, such as in the development of memory devices based on oxides with silicon, where a reaction creating a new material at the interface **[3.3]** would have prevented the resulting device from working. ARTEMIS predicted this effect, *"effectively saving the company £200K"* **[5.3]**. The novel work based on interface design also led to a joint patent for thermoelectric devices **[5.3]**.

Stimulating growth: The collaboration with Deregallera, centred on ARTEMIS, has helped the company to focus and strengthen its technology development programme, establishing itself as a key UK player in this space, securing additional investment (including £3M from the MOD and over £1M from the Faraday Battery Challenge), growing staff numbers from 10 to over 20 and creating jobs in an economically deprived area of South Wales **[5.4]**. Deregallera has recently won a share of the Welsh Government's EU-funded £63.4M SMART Cymru programme that will enable it to commission a pilot production line, the first step in moving from lab-scale materials discovery to commercial-scale battery manufacture.

Beyond Deregalla, ARTEMIS has enhanced the activity of several other SMEs in the area of next generation energy systems. For example, ARTEMIS was used by Solaris Photonics to find the appropriate contacts for an unusual solar cell design **[3.5]** which "*saved the project*" **[5.5]** and allowed the company to go to investors with a working design for their device. Lambda Energy is an R&D start-up that develops spectral converters for boosting the power output of solar panels. The company used ARTEMIS to simulate the interfaces between quantum dots (made from oxide perovskites) and the embedding medium, solving an issue which prevented the quantum dots from functioning **[3.3]**, allowing them *"to secure external funding of £50,000"* from investors and to move forward with the development of spectral converters **[5.6]**. Finally, ARTEMIS is having direct impact with Anaphite who are using it to explore new battery materials. Here, ARTEMIS is being used to design novel multilayer battery materials **[3.5; 3.6]**. As such, the founders of Anaphite have said that ARTEMIS is *"vital to our future success"* **[5.7]**.

Summary statement: The University of Exeter has developed ARTEMIS, a unique theoretical framework and simulation tool developed to explore material interfaces at the atomic scale. Working with several UK based SMEs, ARTEMIS has been applied to solve problems found during the development of next-generation energy systems and storage. The results have focussed R&D activities, attracted additional investment and improved development success. This work has strengthened the UK's technology base in key areas such as energy storage and battery technology, with a financial impact of >£6M garnered through investment and savings to our partner SMEs.

Table 1: Financial impact summary

Company	Application	Impact source	Amount
Deregallera	Capacitive energy storage	Additional funding	£3,000,000
Deregallera	Capacitive energy storage	Cost saving	£2,000,000
Deregallera	Batteries	Additional funding	£958,000
Deregallera	Batteries	Additional funding	£437,000
Deregallera	Memory devices	Cost saving	£200,000
Lambda Energy	Solar cells	Additional funding	£50,000
		Total	**£6,645,000**

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

5.1 Statement from CEO of Deregallera, Martin Boughtwood

5.2 Second Statement from CEO of Deregallera, Martin Boughtwood

5.3 Supporting letter from Peter Curran, Principal Scientist and Head of Materials for Deregallera

5.4 "Our valleys, our future" Welsh Government (2017) [available online]

5.5 Supporting statement from Chief Technical Officer for Solaris Photonics, Monica Saavedra

5.6 Supporting Letter, COO and co-founder Lambda Energy, Mark Brenchley

5.7 Supporting Letter, Anaphite Founders, Alex Hewett and Samuel Burrows