RCloud Tasking Form – Part B: Statement of Requirement (SoR)

Title of Requirement	Accelerating the Discovery of Advanced Energetic Materials using computational chemistry approaches
Requisition No.	RQ00000010147
SoR Version	**1.1**

1.	**Statement of Requirements**
1.1	**Summary and Background Information**
	The Advanced Energetic Materials project aims to accelerate the discovery and delivery of new explosives and energetic materials for future use by UK Defence and Homeland Security. With ever-increasing demands on energetics to meet tougher mission requirements, the UK requires new materials that are able to provide increased performance or else offer other key advantages. In addition, there is significant potential to realise other important benefits – including reductions in both manufacturing costs and environmental impact. This high technical risk, low technology readiness level (TRL) research programme aims to harness new and under-exploited technologies, with a focus on computational processes, for the purposes of identifying new energetic materials, as well as on finding new synthesis pathways – both to those new energetic materials, and to existing ones for which significant barriers to production currently exist. As a critical, underpinning technology, new energetic materials are required for a wide range of defence and security applications. Energetic materials (or 'energetics') are materials with a high amount of stored, but suitably accessible, chemical energy. Foremost amongst these are explosives, propellants and pyrotechnics, with additional examples including energetic additives in the form of binders, plasticisers or bonding agents. Novel energetic molecules, for use in warhead (explosives) and propulsion (propellants) formulations, are the strategic focus for this very low technology readiness level (TRL) research. At present, human-led discovery of new energetic materials through manual practices often relies on decades of research, significant continuous funding, and hazardous 'human-in-the-loop' tasks. The aim of this research stream is to address the need for new energetic materials and mitigate associated risks by developing *in silico* methods. In this way, the project aims to discover and deliver advanced energetic materials (and potentially valuable new precursors to known materials), to meet tightly-defined production and performance criteria.
1.2	**Requirement**
	Dstl's overarching requirement is for the development of energetic materials. This SOR is seeking proposals using computational chemistry techniques to achieve this goal, with desirable outputs including: • Discovery and characterisation of new high-performing molecules or formulations • New, more attainable, precursors • Novel methods that noticeably enhance the established processes towards these outputs The primary metric of higher performance is enhanced energetic effect per quantity of material (e.g. the power-to-weight ratio of an explosive) as this has the potential to limit necessary precursors and generation of waste or by-products through their manufacture. It could also lead to more fuel efficient missiles. Other metrics for performance may also include:

- Good mechanical properties (system-specific and examples might include: elasticity, malleability, ductility, impact strength, fatigue limit, toughness)
- Inexpensive production processes
- More scalable processes that rely on abundant materials
- Improved safety of manufacture and materials
- Reliability in a variety of environments
- Compatibility with a wide array of chemicals
- Environmental compliance

Bids that are perceived as having high technical risk or novelty will be encouraged, and the generation of patents or publications for the benefit of national prosperity will be positively explored. The innovation in proposals will receive specific scoring criteria when assessments of the returns are undertaken.

Please note that Dstl has a duty of care to ensure research is conducted safely under our sponsorship, and that this responsibility is of utmost importance to us.

Whilst not directly expected as part of this requirement, should any practical work involving energetic materials become necessary by the Supplier on the basis that it is deemed fundamental to successful delivery, bids will need to demonstrate sufficient prior experience and suitable capability to work with energetic materials, or else will be rejected. To this end, collaborative bids with partners with the required energetics experience/ facilities are welcomed.

Where sufficient experience and capability to work safely with energetic materials is not demonstrated, practical work must instead be restricted to the study of justifiably representative, non-energetic model compounds and systems only.

Bids will be assessed by a panel which may include Government technical experts from the Centre of Excellence for Energetic Materials (CoEEM) as well as Dstl, using Proposal criteria in Section 5. Communications will be managed through R-Cloud and in accordance with the standard Dstl Commercial process.

After the contract(s) have been awarded, activity will be instigated by the Authority, with a Project Kick-Off Meeting at the agreement of all parties.

Please note that any novel discoveries that offer distinct military advantage may necessitate a significant increase in classification level of this work as the project progresses. Therefore any suppliers who intend to resource PhD students to support contract delivery, need to be aware that a Research Worker Form will need to be completed. Individuals who are eligible (provided they meet the requirements of the checks) are from the following list:

- UK nationals
- Irish citizens
- From the EU, EAA, or Switzerland and has the appropriate EU Settlement Scheme status to study and/or work in the UK at the organisation detailed
- from outside the UK, the Republic of Ireland, EU, EEA or Switzerland and has the appropriate immigration status (in accordance with the requirements of the UK Visas & Immigration) to study and/or work in the UK at the organisation detailed
- not going to be studying or working in the UK

Discovery & Characterisation via Computational Chemistry

The discovery and characterisation of energetic molecules via computational chemistry is an emerging field of wide interest [1] [2]. Dstl is seeking proposals that aim to develop methods using *ab initio*, molecular mechanics or other computational techniques to predict the performance and

	properties of energetic materials. Proposals are welcome for techniques and outputs that either encompass a variety, or a specific class, of energetic materials. Dstl seeks proposals in any or all of the following areas: • Identification and characterisation of high-performing energetics and other relevant properties using computational methods. • Development of existing and/or new methods for theoretical energetic prediction and development. • Development of existing and/or new methods for crystal packing and density predictions of energetic molecular systems, to screen for performance and/or material model generation. **<u>Indicative Budget</u>** The Authority has currently identified confirmed funding of £500K (EX VAT) with £200K available in FY 22/23 and £300k available in FY 23/24, however these figures are purely indicative, and bidders are invited to submit costed proposals above these figures as the Authority may be able to secure additional funding prior to award of any Contract. Please also note that the Authority may place more than one contract as a result of this competition, therefore please note that bids that do not maximise the full funding availability will be considered as well as those that maximise availability of funding for each FY. Please also note that PhD proposals will also be considered for this ITT. Proposals for these should include firm price and breakdown as appropriate for a three year PhD. **References** [1] Computational Chemistry: The Fate of Current Methods and Future Challenges (2017) - https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201709943 [2] Structural Characteristics and Reactivity Relationships of Nitroaromatic and Nitramine Explosives (2007) - https://www.mdpi.com/1422-0067/8/12/1234/htm
1.3	**Options or follow on work**
	Two year contracts are offered. Options for follow-on work in Year 3 will potentially be available, subject to technical review of Yrs 1 & 2 outputs. Follow on work could for example include practical support, etc., subject to agreement between DSTL and the supplier at the end of Yr2. If PhDs are submitted in Year 1 this would be supported throughout the 3-4 year standard period. **<u>The Authority shall not be obliged to exercise these options.</u>**
1.4	**Contract Management Activities**
	All successful bids, after contract award will be initiated by a Project Kick Off Meeting organised by the Authority. It is expected that kick off meetings will be scheduled in promptly after contract award. Deliverables will be managed by the Authority and expected to the timescale as outlined in Table 1.6 At Contract Closure, a wash up meeting will be delivered to discuss next steps, recommendations and feedback, which will be captured by the Dstl Project Team.

1.5	**Health & Safety, Environmental, Social, Ethical, Regulatory or Legislative aspects of the requirement**
	All work is to be performed in compliance with relevant UK legislation (including H&S). See also the Requirement (section 1.2) for information relating to Dstl's duty of care when sponsoring work involving energetic and/or potentially energetic materials.

1.6	Deliverables & Intellectual Property Rights (IPR)					
Ref.	**Title**	**Due by**	**Format**	**Expected classification (subject to change)**	**What information is required in the deliverable**	**IPR Condition**
D – 1	Progress meeting	T+3, T+6, T+9, T+12, T+15, T+18, T+21 months.	Presentation from Supplier (remote or in-person meeting)	UK OFFICIAL	Presentation to Dstl project team, to include: • Update on technical progress • Commercial aspects • Review of deliverables • Risks/issues • GFA and supplier performance • Technical presentation/knowledge share sessions detailing any methods, techniques and other areas of technical interest to support understanding and learning amongst DSTL staff.	DEFCON 705
D - 2	Year-End Report	T+12 months	Report	UK OFFICIAL	Full year-end report, to include: • Project background • Summary of Yr1 work • Conclusions • Recommendations for follow-on research, with plans for following year	DEFCON 705

					• Identification and summary of IP (potential or actual) arising in-year. • Progress versus deliverables Recommendations for any potential parallel research	
D - 3	Final report	T+24 months	Report & presentation	UK OFFICIAL	Full final report, to include: • Project background • Summary of Yr1 & Yr2 work • Conclusions • Recommendations for follow-on research • Copies of relevant publications arising or pending • Identification and summary of IP (potential or actual) arising • Progress versus deliverables • Any other technical issues or findings that Dstl should reasonably be made aware of Additional presentation, to include: • Brief summary of each year's work	DEFCON 705

					• Overall progress and conclusions • Demonstration of system and/or technology outputs • Recommendations for future work • Summary of publications and IP (submitted or pending) arising	
D – 4	Supporting files, outputs and documentation	T+24 months	Input files, Output files, YAML files etc.	UK OFFICIAL	Files (e.g. inputs and outputs), supporting documents for any software, code or method used for any relevant work done under this research. To be able to recreate the outputs and enable further exploitation of methods and techniques.	DEFCON 705

1.7	**Deliverable Acceptance Criteria**
	All deliverables to be emailed to: Redacted under FOIA exemption Stakeholder presentation deliverables to include attendance of meetings with Dstl and delivery to key stakeholders. All material intended for external publication to be emailed to Redacted under FOIA exemption for technical review. If any published papers include GFI, Dstl must have sight of them and must provide permission to publish prior to the papers being shared.

2	**Evaluation Criteria**
2.1	Method Explanation

The Tender evaluation utilises an absolute method, whereby a Value For Money (VfM) Index is applied to identify the preferred bidder. This approach divides the total score of the non-cost (Technical) criteria by the tender cost. It ranks tenders on the quality (represented by the non-cost score) for each £ (or £k or £m) of cost.

An illustrative example is outlined below for reference purposes only:

Tender	Non-Cost Score	Cost (£)[Thousand]	VfM Index Score	Rank
A	62	20	3.10	3
B	85	24	3.54	1
C	100	29	3.44	2

2.2	Technical Evaluation Criteria

The technical evaluation shall be scored on the following questions, noting that any proposal that is marked as a Fail against Serial 1 or 2 shall not be considered for task award.

Serial	Question	Weighting	Score
1	The proposal provides a clear and unambiguous statement which meets the technical requirements in the Statement of Requirement.	N/A	Pass / Fail
2	The proposal demonstrates sufficient prior experience/provenance of the applicant's organisation and/or Principal Investigator in the relevant technical fields (at an internationally publishable standard or any other equivalent indication of skills and knowledge), to be able to undertake the proposed work.	20	0,3,4,5
3	The proposal demonstrates the existence of suitable experimental facilities or assets, either in the home capability or allied/accessible labs for example, to be able to undertake the proposed work.	20	0,3,4,5

4	The proposal is based on and demonstrates a suitable level of novelty/innovation.	20	0,3,4,5
5	The proposal clearly demonstrates how the outcomes will be delivered and the work completed	20	0,3,4,5
6	The proposal outcomes demonstrate impact for the UK Energetics sector.	20	0,3,4,5

The technical questions shall be assessed and marked using the following scoring definitions

Definition	Characteristics	Score
Excellent	The response addresses all elements of the requirement, and provides a comprehensive, unambiguous and thorough explanation of how the requirement will be fulfilled.	5
Good	The response addresses all of the elements of the requirement and provides sufficient detail and explanation of how the requirement will be fulfilled.	4
Adequate	The response addresses the technical elements of the requirement but is weaker in some other areas and does not fully detail or explain how the requirement will be fulfilled which may require clarification.	3
Fail	The response does not address or explain how the requirement will be fulfilled and or fails to demonstrate the ability to meet the requirement.	0

Under the Technical Evaluation the maximum available weighted score is 1000, under the VFM Index this score (Non-Cost) shall be divided by the cost of your proposal to generated the VfM Index Score.

2.3 Commercial Evaluation Criteria

The commercial evaluation shall be assessed against the following Pass / Fail questions. Please note, a fail against any of the commercial questions will result in your proposal not being considered for Technical Evaluation.

Serial	Question	Score
1	The proposal has been submitted as a firm i.e. non-variable price for the proposed two year duration (except if a PhD is being offered as a solution, in which case it should be priced for the entire proposed duration of the PhD topic).	Pass / Fail
2	The Tenderers proposal includes a completed RCloud Part C Task Response Form and a suggested milestone payment plan, with payment milestones linked to deliverables. Not all deliverables need be associated with a payment milestone.	Pass / Fail
3	The proposal prices do not exceed the R Cloud Rates submitted upon application and acceptance.	Pass / Fail
4	Cyber Security - the Tenderer has completed a Supplier Assurance Questionnaire demonstrating their compliance with the LOW Cyber Security Controls detailed in DEF STAN 05-138. If the Tenderer is unable to demonstrate compliance at ITT return, then the Tenderer must provide a draft Cyber Implementation Plan (CIP) detailing the steps they will take to meet the Controls.	Pass / Fail
5	Completed Research Worker Form (Dstl Form 388) for all Contractors personnel undertaking Research and	Pass / Fail

		Development activities under this requirement or details of individual SC Clearances held where appropriate.		
	6	The Supplier submits a priced Commercial proposal (Qty 1) and an unpriced Technical Proposal (Qty 1).	Pass / Fail	
	7	The proposal accepts the Additional Terms and Conditions laid out in RCloud_Tasking_Form_Part A-Task_Overview	Pass / Fail	