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

Title of Requirement	Computational modelling of carbon materials for hypersonic applications
Requisition No.	**RQ0000027002**
SoR Version	**1.5**

1.	**Statement of Requirements**
1.1	**Summary and Background Information**
	Previous Dstl studies has shown the potential for insight and guidance to the development of materials for thermal protection systems using modern computational methods including electronic structure calculations to predict material structures at the atomistic level, material properties (such as thermophysical properties like thermal conductivities) and the mechanisms of elementary reactions. Modelling allows interpretation of experimental results and can accelerate the development of new materials but previous modelling initiatives have been hampered by the lack of practitioner skills. Phase 1 – Dstl requires the development of a modelling strategy and capability roadmap for the first principles prediction of thermos-sphysical properties of carbon materials used for hypersonic applications. This requires a supplier with recognised expertise in materials modelling to work with and support the Dstl Technical Partner through meetings and workshop activities. The key output from Phase 1 will be a report detailing the modelling strategy and capability roadmap. In Phase 2, the approaches described in the literature and explored in previous Dstl funded modelling work to understand the basic properties of carbon materials (atomistic structure prediction and the calculation of properties of materials from these structures) will be developed further and applied to simple structures. Where possible, results will be validated by comparison with experimental results or other modelling. Subsequently, more complex materials will be simulated. Phase 3 will address the pyrolysis of the model structures used in Phase 2 by simulating the temperatures and pressures to which real materials are subject in hypersonic applications **Overview** Initially, the supplier will be contracted to fulfil the Phase 1 requirements for the project, with options for Phases 2 and 3 to be contracted with the same supplier.

	Phase 1: Feasibility study- calculation of thermo-physical properties of carbon materials for hypersonic applications (T-PPMHAs) Review previous work, develop modelling strategy and code requirements and agree with the Dstl HTTPS technical lead: • the requirements, timescale and technical roadmap to create a modelling capability to predict thermal conductivities of carbon materials for hypersonic applications; • the support to be provided to Dstl staff to develop expert practitioner status in computational materials science. **Review & Decision Point** PTA to review the Recommendations from the Phase 1 feasibility study and decide whether to proceed to Phase 2: decision criteria – feasibility, required resources, value of computable information and timescales. **Phase 2: Calculation of T-PPMHAs at atmospheric temperature and pressure for selected materials agreed with PTA** Subject to successful Customer endorsement / funding, follow-on work will calculate and interpret thermophysical properties of carbon materials for hypersonic applications. **Review & Decision Point** PTA to review the results from the Phase 2 computational study on T-PPMHAs and decide whether to proceed to Phase 3: decision criteria – feasibility, required resources, value of computable information and timescales. **Phase 3: Calculation of T-PPMHAs at different temperatures and pressures for selected materials agreed with technical lead** Following agreement with the technical lead on materials to be modelled, perform and interpret calculations to simulate the effects of temperatures and pressures similar to those experienced by deployed materials and compare with available experimental data.
1.2	**Requirement**
	Phase 1: Development of a modelling strategy and capability roadmap to calculate the thermal conductivities (κ) of a range of materials relevant to the development of materials for hypersonic applications such as, but not limited to, bulk graphite, nano-crystalline graphite, isotropic graphite, amorphous carbon and phenolic resins.

	1. Review previous relevant modelling activities undertaken by Dstl 'in-house' and by its suppliers to develop atomistic models, e.g. for graphite and diamond (from previous Dstl work available as GFI) and phenol-formaldehyde resin (from previous University of Surrey work available as GFI) from which thermophysical properties and chemical properties were calculated at different levels of approximation; 2. Where they do not exist, create atomistic models of carbon materials such as amorphous carbon; this could involve exploitation of pair distribution function measurements expected to be available during the lifetime of this contract (and available as GFI) obtained using the Diamond Light facility; 3. At a time to be agreed with the technical lead (towards the end of the feasibility study), propose, and agree with the Dstl HTTPS technical lead, tractable computational schemes for Phase 2 studies using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), or other, software to compute the thermal conductivities (κ) and (isotropic / non-isotropic) heat flows (J_I, I = X, Y or Z); 4. Propose, and agree with the Dstl HTTPS technical lead, details of the materials to be modelled in Phase 2. Materials to be modelled initially must include simple compounds (such as graphite or diamond) to allow validation by the Supplier together with the PTA of the modelling approach used. Subsequent materials to be modelled could include heterogeneously layered graphite-like materials and must include amorphous carbon and phenol-formaldehyde resins; 5. Providing technical materials modelling consultancy to Dstl members of staff to develop in house Dstl capabilities for a range of materials modelling activities; **Review & Decision Point** 6. Technical lead to review the Recommendations from the Phase 1 feasibility study and decide whether to proceed to Phase 2: decision criteria – feasibility, required resources, value of computable information and timescales.
1.3	**Options or follow on work** *(if none, write 'Not applicable')*
	Phase 2: Calculations of thermophysical properties of materials for hypersonic applications: 1. Apply the approaches agreed in Phase 1 to: a. Models of bulk and layered materials (including, but not limited to, graphite, nano-crystalline graphite, isotropic graphite and phenol-formaldehyde resins) for validation. Validate by comparison with experimental data from the literature and developed from other Dstl studies (available as GFI);

	b. Simulate the effects on the thermal conductivity, κ, of residual water from resin synthesis in the resin structure; c. Simulate the predicted heat flow, J_l, in the different resin models to predict whether this is non-isotropic; 2. Create a set of fragment / crystal structures with different orientations to the incident heat flux; a. Simulate various thermodynamic properties of a single layer of unit cells as a function of the unit cell structure; b. Embed the unit cells in phenol matrix and repeat simulation of thermodynamic properties; c. Increase the complexity and depth of the model by creating layers of differently orientated fragments in the model space, with and without the phenol matrix. Calculate the thermodynamic properties similarly to the single layer; 3. Propose, and agree with the Dstl HTTPS lead, tractable computational schemes using public domain software (e.g. LAMMPS, ABINIT, etc.) to allow the simulation of the graphitization of materials for hypersonic applications when subjected to the temperatures and pressures of real materials in deployed conditions. **Review and decision point** **4.** Technical lead to review the results from the Phase 2 computational study on T-PPMHAs and decide whether to proceed to Phase 3: decision criteria – feasibility, required resources, value of computable information and timescales **Phase 3: Simulation of the graphitization of materials for hypersonic applications** Perform and interpret / compare to experiment pyrolysis simulations using model materials agreed with the Dstl HTTPS lead.
1.4	**Contract Management Activities**
	Meetings as outlined in '1.6. Deliverables and Intellectual Property Rights (IPR)' below
1.5	**Health & Safety, Environmental, Social, Ethical, Regulatory or Legislative aspects of the requirement**
	Normal office environment health & safety (screen display assessment, no hazardous materials or working practices expected)

[redacted]

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	Kick off meeting	T0	Presentation	[redacted]	*Presentation to include but not limited to:* • *Proposed schedule and structure of study.* • *Review of risk management plan.* • *Commercial aspects.* • *Review of deliverables.* • *Risks/issues.* • *GFA and supplier performance*	As per R-Cloud Ts&Cs
D - 2	Fortnightly progress meetings over MS Teams or telephone	T0+2n weeks	Presentation	[redacted]	*Presentation pack to include but not limited to:* • *Update on technical progress* • *Progress report against project schedule.* • *Review of risk management plan.* • *Commercial aspects.* • *Review of deliverables.* • *Risks/issues.* • *GFA requested*	As per R-Cloud Ts&Cs

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D - 3	Interim report / Payment Milestone [redacted]	By 10th March 2023	MS Word or Powerpoint or PDF	[redacted]	*A summary of the work which the supplier has completed at risk; the report must include:* • *A brief review of current approaches to relevant materials modelling* • *Assessment of weaknesses/errors in previous published work using LAMMPS* • *Necessary features of models for further study in Phase 2* *Overview of possible computational schemes to evaluate thermal conductivities and heat flows*	As per R-Cloud Ts&Cs
D – 4	Final report ' Payment Milestone [redacted]	By 24th March 2023	MS Word or Powerpoint or PDF	Official	*Report to include but not limited to:* • *Summary of study findings* • *Proposed models for further study in Phase 2 if funded* • *Proposed computational schemes to evaluate thermal conductivities and heat flows in agreed model(s)*	As per R-Cloud Ts&Cs

					Summary of materials down selected together with technical lead for further modelling in Phase 2, if funded, together with rationale for choice.	
D - 5						

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1.7	Deliverable Acceptance Criteria
	Milestone payment invoices should not be submitted until the deliverable has been accepted in writing (email) by Dstl.
1.8	Government Furnished Assets (GFA)

GFA No.	Unique Identifier/ Serial No	Description:	Available Date	Issued by	Return Date or Disposal Date (T0+)
GFA-1		16 reports generated in previous Dstl funded work at University of Surrey. Files located at [redacted]	T0	PM	Return date T0 + 2

2	Evaluation Criteria
2.1	Method Explanation
	Please submit two versions of your proposal. The Technical proposal should not contain any pricing information. The Commercial version should be a full response to the ITT including both Technical and pricing information. The supplier's proposals will be evaluated by the Dstl technical and commercial authorities to assess whether the content meets with Dstl's requirements and represents appropriate value-for-money. The placing of any contract will depend upon consideration of the proposal received and the Authority reserves the right, at its sole discretion, to proceed to contract for any part or all of a

	suppliers proposal. And if necessary, not to place any contract as a result. Please note the MOD operates a policy of No Acceptable Price No Contract (NAPNOC).
2.2	Technical Evaluation Criteria
	The supplier's proposal will be technically acceptable if considered by Dstl Subject Matter Experts (SMEs) that the plan is credible and it provides sufficient confidence that it will achieve the requirements within the stated timescales.
2.3	Commercial Evaluation Criteria

Commercial Proposals will be assessed as to whether the content meets with Dstl's requirements and represents appropriate value-for-money.

Commercial Compliance:

Firm price and full firm price breakdown for all costs to be incurred to fulfil this requirement, including:

- What rates are being used for what role
- Quantity of manpower hours per role
- Any Materials costs
- Any Facility costs
- Any sub-contractor costs
- Any travel and subsistence costs
- Any other cost

Compliance with this Task specific terms and conditions as stated within the Statement of Requirement and respective Call-Off Tasking Form.

Commercial Scoring criteria:

Score	Definition
Pass	Fully meets the Authority's requirement. Provision and acceptance of the sub-criteria information in the format requested, which is clear, unambiguous and transparent.
Fail	Unacceptable/Nil Return. Tenderer did not respond to the question or the response wholly failed to demonstrate an ability to meet the sub-criteria requirement