

Computational Sciences in Energy Research

Summary

Shell and NWO propose to start a large scale PPP in basic research within the Topsector Energie. NWO and Shell intend to invest 21 and 24 M€ in cash, respectively. While the axis NWO-Shell is central, other firms will be explicitly approached to join and invest in this collaboration.

This collaboration is a scientific research programme for existing and alternative energy sources. The lion's share of the Shell investment comprises Computational Sciences (CS) for energy research, the results of which are enabling for all innovation tables in the Topsector Energie and other Topsectors. Another part is specifically aimed at Sustainable Energy that has direct links to one of the Innovation tables. A Steering Committee to shape and manage this collaboration as one programme has already been formed together with NWO and is proposed to be extended to include a representative of the Energy Topteam. FOM Foundation (part of NWO) executes the programme. This large-scale PPS has a distinct added value for all parties involved, including the Innovatietafels in the Topsector Energie, that would not be possible through other schemes.

Objective

The programme aims at an extensive long term collaboration covering a range of scientific disciplines (physics, chemistry, engineering sciences, mathematics, computational sciences) for exploitation of alternative and existing energy sources. The collaboration consists of a large cash investment in a research programme and in research infrastructure that should lead to:

- a) an overarching PPS, at the knowledge base of the entire Topsector Energy, feeding the *innovatietafels* with new knowledge, in particular we mention Solar Fuels and Smart Energy Grids;
- b) a large boost to create a firm Computational Sciences foundation in the NL with impact on the Energy sector and potentially other sectors;
- c) to enhance the capabilities of NL based multinational Shell of its Shell Technology Centre Bangalore (STCB).

Parties in this Collaboration

Funding parties	Collaborating parties
Shell	Alliander (also funding part of the collaboration)
NWO + divisions (incl. FOM)	Currently talks with DSM, Nuon, others
Universities (in kind)	Potentially all universities and NWO institutes

The program

The entire Shell-NWO collaboration encompasses Computational Sciences in energy research and a specific activity in sustainable energy. The results are relevant for the improved exploration and recovery of oil and gas and are enabling to other innovation tables of Topsector Energie, e.g. new algorithms that improve operations of smart grids, modelling of the CO₂ sequestration process, or new concepts in battery technologies.

The entire collaboration is managed as one programme and is completely executed in the Netherlands. It consists of two parts:

A) Computational sciences with relevance for enhanced oil and gas recovery, comprising themes like 'flows in nanopores', 'materials science', en 'very large inversion problems'. Shell wants to strengthen its capabilities in STCB. Therefore it wishes to educate Indian students in the Netherlands according to the 'Dutch Standard' and offer them employment in Bangalore after their PhD in the NL. Shell will create a large Excellence Pool consisting of a selection of the best students from India (and possibly others). From this Excellence Pool NWO project leaders can draw their candidates.

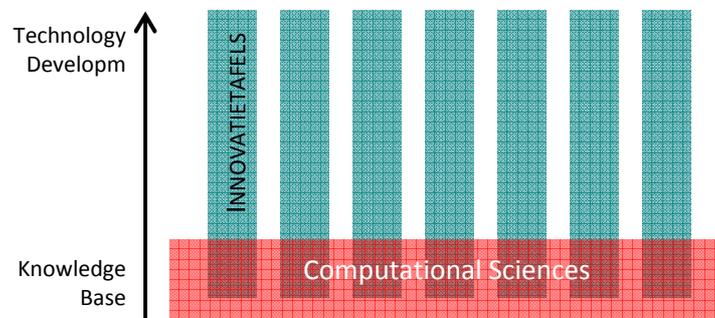
This investment in talent and infrastructure will lead to an increase in quantity and quality of the CS research in the NL.

B) Sustainable Energy, comprising the themes 'uncertainty reduction in smart energy grids', and 'solar fuels'. This theme is part of a larger NWO theme 'Sustainable Energy', which is open to other industrial participation, hence considerable spinoff to other sectors can be expected upon entering of new industrial partners. Currently Alliander has indicated its interest in Solar Fuels and has the intention to contribute M€ 1,0, while other parties are being approached, like DSM and Nuon. The topics mentioned above are fundamental in nature, aimed to build up a strong knowledge base.

Fit to Topsector Energie

Due to the inherent cross-disciplinary approach, the generic character of the CS programme, and the fact that Shell wants to invest the 24 M€ in one coherent programme we propose to construct an overarching PPP, at the knowledge base of the entire sector, feeding the *innovatietafels* with new knowledge, or potentially leading to new *innovatietafels*.

Considering the topics, this proposal relates to several *innovatietafels* within topsector Energie (Zon, Smart Grids, Energiebesparing in de industrie, Gas and Wind). Cross fertilisation and exchange between *innovatietafels* will occur through science and technology workshops across the Topsector, see below.



Governance & Legal structure

The entire collaboration will be governed by a Steering Committee consisting of members from Shell and NWO (already established), extended with a member of the Topteam Energy.

A programme committee consisting of esteemed scientists from academia and industry will assess the research framework and formulate the scientific challenges and will be instrumental in workshops and network activities.

This collaboration will be placed under Foundation FOM. FOM represents the physics division of NWO and has a legal status as independent 'Stichting'. FOM will be the central organising, employing, managing and administrating office. Shell, with many other companies, and FOM have a long standing tradition in collaborations and FOM has been very successful with its Industrial Partnership Programme, currently managing public-private research partnerships with a portfolio of M€ 50.

A programme coordinator from the Industrial Partnership Programme will manage the programme including administrative support. He is responsible for knowledge transfer and connection to the innovation tables and will act as secretary to the Steering and Programme Committee.

Shell, NWO, and FOM will sign a consortium agreement arranging the legal, IP, personnel, knowledge transfer, and other affairs.

Knowledge transfer and Intellectual Property

Due to the range of possible topics expected in the projects, it will be assessed in time which projects have a connection to which innovation table. Accordingly, these projects will be part of the particular consortium and will take part in programme meetings to exchange and share knowledge. In this way knowledge transfer is optimal.

This programme strives to maximise the transfer of knowledge within the Topsector Energie and beyond. Shell and NWO will draw up an IP arrangement that does justice to the intent that third parties have access to IP.

Coherence

Despite the huge size of the programme it will be feasible to maintain the needed coherence:

- the interaction between the disciplines in the programme through progress meetings, workshops and network activities;
- connection to the activities and themes of the Topsector Energie via thematic conferences and cross-Topsector activities;
- the interaction with STCB through the excellence pool and active exchange and interactions during the programme by organising workshops, stages, guest scientists, in Bangalore and vice versa;
- FOM as executive management office is also employer of all research personnel, which greatly facilitates coherence.

Budget

The total budget of part A amounts to 33 M€ and of B) to 18,5 M€. The overall Shell investment is 24 M€ in-cash, divided over 20M€ in part A (Computational Sciences) and 4M€ in part B (Smart Energy Grids and Solar Fuels). The requested NWO investment totals 21 M€ in-cash, divided over part A and B according to a split which will be defined in the coming weeks. Next to that an in-kind contribution by universities is requested. Other companies are likely to join this consortium and will contribute in cash. NWO has already committed a large share of its contribution on the precondition that Shell also invests the requested budget, which, in turn, depends on the successful incorporation in and approval of the innovation contract and the related fiscal benefits.

Scientific spin off

About 60 research projects in fundamental computational sciences and 15 in sustainable energy are financed next to a considerable investment in knowledge infrastructure. While the Indian PhD students will move back to India after their PhD, what remains are the strong CS foundations and an organised and internationally visible scientific CS community. The scientific results (new algorithms and models) will most likely have spill over to other research fields like medicine, particle physics, meteorology, etc.

Economic spin off

By executing this programme in the NL the Dutch economy will benefit due to the foundations in CS that arise from this programme with potential knowledge transfer to energy and other technology sectors. In particular, Shell is a large employer in NL; also for their capabilities in Rijswijk and Amsterdam a good scientific home base with access to highly educated potential new employees and a strong scientific infrastructure and network, is important. This naturally holds for other NL based industries. This programme helps to keep NL an attractive location for Shell.

Overview added value involved parties

Due to the size and the structure of the PPS, described in this proposal and managed as one program, there are some clear benefits, that, together, would otherwise be difficult to obtain. These are:

- 1) Investment at the knowledge base of the Topsector Energy across the *innovatietafels*.
- 2) Long term benefits: major increase in fundamental CS research budget of NWO invested in talent and infrastructure; what remains after the PhD students return to India are the CS foundations (the knowledge infrastructure and new CS positions at universities) on which new CS initiatives can build. Also durable relations between NL and India, one of the BRICS countries, and in particular STCB are established.
- 3) Enhancement of the capabilities at Shell Bangalore through talent development according to the 'Dutch Standard';

Enlisted here is the added value for the different stakeholders.

Stakeholder	Added Value Program
Shell	<p>Education of Indian graduates up to Dutch PhD standards in CS to be recruited for STCB.</p> <p>Single point managed (NWO/FOM) program for Indian trainees.</p> <p>Linked in to Topsector Energy Programs, access to IP in a wide array of technology.</p> <p>Tax relief via a TKI construction.</p>
NWO + divisions	<p>PPS with excellent fundamental research projects selected based on NWO standards.</p> <p>Development of Dutch knowledge base for (sustainable) energy.</p> <p>Development of Dutch knowledge base for computational sciences.</p> <p>Modest investment leads to huge increase budget for fundamental CS research.</p> <p>Ability to participate in a large multidisciplinary program.</p> <p>Entrance to Indian science community.</p> <p>Chance for NWO to develop collaborations with one of the BRICS countries.</p>
Knowledge Infrastr./ Universities	<p>Building up the foundations of CS in the Netherlands in chairs (talent) and in physical infrastructure.</p> <p>Cross-fertilization to other areas like medical, meteorology, particle physics, process technology, etc.</p>
Dutch CS field	<p>Organization and profiling of the entire CS field in the NL, this is a clear need.</p> <p>International visibility and chance to attract investments from abroad, e.g. a CECAM node in EU framework.</p> <p>Potentially new prominent and visible leading scientists in CS.</p>
Dutch economy	<p>When the foundations are laid the CS development at large in the NL may attract new talented scientists.</p> <p>Due to the generic character of this program it may impact development of other areas like battery technologies, CO2 storage and conversion, traffic simulations, medical image processing, ...</p> <p>Investments in both fundamental as well as applied computing sciences in US and China have already led to considerable innovations. This program is uniquely positioned to achieve that.</p>
Topsector Energy	<p>Substantial <i>in cash</i> support to the Topsector initiatives via a multidisciplinary TKI.</p> <p>Program enabling all <i>innovatietafels</i> through investment in knowledge base via CS.</p>
Topsector Chemie Topsector HTSM Topsector ICT	<p>Computational Chemistry is part of this programme.</p> <p>Computational materials science is part of this programme.</p> <p>Substantial connection to the Topsector ICT .</p>

Status

Shell, NWO and FOM have formed a steering committee to show their commitment and give shape to this collaboration. In a first meeting the committee has laid out the contours of the programme.

NWO has already committed the requested budget. Applicability of the RDA+ arrangement is a precondition for Shell to continue this collaboration.

Connecting Computational Sciences with the Topsector Energy TKI's

Purpose

Due to its interdisciplinary nature, the Computational Sciences Program will strive for proper embedding in several Topsectors, but primarily in the Topsectors Energy, Chemistry and High Tech Systems.

Embedding will be realized by involving the relevant innovation tables in the programming of the research projects by means of a number of open calls for proposals and by participation of TKI representatives in ad hoc program committees.

Selection of the proposals will occur on the basis of thematic fit to the call, the subsequent selection of the full proposals will take place on the basis of excellence and budgetary space available. In this way research projects of the CS program will be linked to TKI's in which Computational Science plays an enabling role whilst ensuring that the overall program continues to align with the priorities set by the Topteams.

Projects will not be upfront assigned to the Innovation Tables.

During the execution phase selected projects will be embedded in the relevant TKI schemes, wherein also other parties will be involved, enabling optimal knowledge transfer.

Separate TKI?

While the program was initially proposed as a separate TKI, this is not essential. Essence is that the initiative qualifies for RDA+ for its members. If the Topsector Energy decides to go for one encompassing TKI, including this program, that is perfectly acceptable. It would even simplify the organization and make it easier to connect to the innovation tables.

Thematic Fit

No detailed discussions have been held with all TKI's so far, but on the basis of preliminary engagements opportunities are foreseen at the following tables/roadmaps (the initiative has already been mentioned in the innovation contracts Wind, Smart Grids and Solar):

- Gas
- Energy Savings in the Industry
- Smart Grids
- Wind
- Solar Energy (in Energy and HTSM)
- Materials (in HTSM and Chemistry)
- Solar Fuels (also in HTSM)
- ICT

Governance

We propose the following process to ensure the proper linkage between the CS program and the Energy TKI's whilst ensuring that the overall CS package aligns with the objectives/priorities of the Energy sector:

A. Workshop

There are a number of alternative ways to match demand, supply (and, linked to this, competence). Proposal is to adopt the 'call' system as a starting point, in line with the objective to move to a demand-driven innovation program. There will be 5 calls throughout the program, linked to a specific TKI or set of TKI's, selected by the CS Program Committee. Prior to each call, TKI representatives and the CS Program Committee will define in a workshop the technical challenges for the TKI in relation to computational sciences and the priorities/size of the CS program in relation to potentially other enabling TKIs. They will form the basis for the formulation of broad scientific challenges, allowing the submission of a broad and cross-disciplinary range of proposals.

B. Call for pre-proposals based on the Workshop Challenges.

The Call will be written and launched by an ad hoc extended Program Committee (the regular PC plus 1 representative of Topteam Energy (in case Energy-assigned NWO funds are involved) and 2 TKI members (initially from Energy, but could be extended to other sectors).

C. Pre-proposal Matching

The matching will be carried out by the extended PC. Selection on the basis of: Fit to the theme of the call and innovative character and the overall criteria set for Energy. Those proposals where there is a strong demand-supply (competence) match will be worked out in a full and more detailed program line..

D. Selection full proposals.

Confirmation of full programs will follow the regular NWO procedures and excellence criteria.

E. Execution

The researchers in the projects will be embedded in the projects and programs in the TKI/roadmap that is subject of the call in order to ensure optimal knowledge transfer.

Examples of CS themes

A number of examples of CS themes, which have a fit with the Energy TKI's are given below:

- Development of better seismic interpretation techniques for geological layers which are at this moment not explored (shallow or shale gas, requiring higher resolution, i.e. more computing power).
- Modeling of hydraulic fracturing in shale gas development, requiring combined models of hydrodynamics, geomechanics, thermodynamics and chemistry.
- For process technology CS is of growing importance. Black and white box modeling of unit operations, process design and modeling of multi-phase flow in complex environment are some examples of relevant applications.
- Smart grid optimization schemes
- Smart material design optimization
- Design of better catalytic reactions