

Publishable executive summary

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The task will be accomplished through the integration of molecular modelling in rational design process, considering main aspects which characterise the development of novel materials: characteristics expected components to gain the desired properties, technologies available to process materials.

In a context of sustainability, up-grading post industrial rejects goes beyond simple re-use and aim to obtain eco-designed materials from sources that actually represent a production cost and are a waste problem.

Through nanoparticles embedding, polymers matrices reach high level of competitiveness towards raw materials.

Project will investigate aspects regarding micro-nano phase behaviour of matrices themselves, interfaces between nanomaterials and matrices to obtain thermal resistance and stability, combined with transparent aspect and mechanical resistance, which are basic for the applications named before.

Project will explore also how injection moulding, extrusion and fibre spinning technologies can respond to the need of an economic way to process novel composites.

Consortium

The partnership is widely trans-national, combining 4 industrial partners (SMEs), 2 industrial research centres and 4 universities research departments from 6 different Countries (Italy, Sweden, Spain, Poland, Slovenia and Israel). It is unlikely that a consortium with all necessary skills could have been formed within a single country.

The partnership is vertically integrated as it contains raw materials and rejects suppliers, technology developers, lighting, automotive building and textile manufactures as end users.

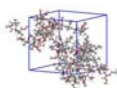
The partnership is highly complementary and has the necessary skills and facilities to carry out the allocated workpackages.

Cooperation among members will continue to interact both technically and commercially at the end of the proposed programme.

Co-ordinator contact details follows:

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CONSORTIUM OVERVIEW				
No	Name	Country	Main mission or business activities	Skills and contribution
1	CRP	IT	Industrial research centre - plastic material, optics and nanotechnology	Project co-ordinator , automotive industry experienced in development and production, rejects material provider
2	IFP-SICOMP	SE	Research centre – polymers, fibres, textiles, composites	Expert in fibre spinning technology
3	UNITS	IT	Higher education - research in computational chemistry	Material modelling Scientific and academic dissemination
4	LTU	SE	Higher education - research in polymeric composites	Materials characterization
5	WUT	PL	Higher education - material research	Fundamental research, material compatibilization (nanopowders) and characterization. Socio- economic aspects
6	UPV-EHU	S	Higher education - research in polymeric chemistry	Fundamental research, material compatibilization (nanoclay)
7	NPI	IL	SME – nanofillers production	Nanofillers provider
8	M&P Burja	SL	SME - polymers extrusion	Expert in extrusion technology, rejects material provider
9	GP	S	SME - polymers sheet producer	Expert in sheets technology, rejects material provider
10	POLY	IL	SME - nano material developer	NanoTechnology developer Industrial dissemination

Project objectives

The technical objective of the proposed project is to up grade post industrial rejects (mainly PC, PMMA and ABS) in order to obtain new high added value materials, extending in that way, the life cycle of the materials diminishing their environmental impact. Special emphasis will be put to achieve:

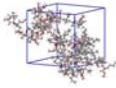
- **thermal stability** of the nanocomposites: over 180°C and in some case preferably around 250°C
- **mechanical properties** an improvement of 30% at least is expected vs rejects
- **transparency** same as in virgin materials (around 90% of transmittance)

Depending on final product and technology such properties could be increased using nanoclay and/or nanopowders.

On the other hand we intend to use nanofillers as process aid in order to increase mouldability of rejects materials. In re-processing of polymers physical properties are deteriorated, so it is expected that the nanofillers, (such as nanocalcium carbonate) will have a useful impact in the recycling process.

The first scientific objective is to develop a rational eco design method through:

- integration of molecular modelling in industrial approach



- development of modelling procedures suitable for polymeric blends/nano composites coming from post-industrial rejects based on commercial SW
- modelling procedures validation

Success in reaching the first scientific objective will be tested by month 30, milestone M2.3 Validation of models.

The second scientific objective is related to the embedding of nanoparticles and new materials preparation: MOMO will apply melt intercalation for the production of nanocomposite recycled materials based on nanoclays. Melt intercalation represents a great goal because of it can be a cost effective way to produce materials based on scraps, moreover it has already been used to produce nanoclay-nanocomposite materials

MOMO will keep a strong effort in developing a suitable technique to embed nanoparticles in polymers matrices. In particular two approaches will be followed:

- 1) nanoparticles will be dispersed in to virgin materials first, and post industrial rejects secondly, making use of extrusion compounding
 - 2) “in situ” polymerisation to obtain homogenous dispersion of nanoparticles into virgin polymer/co-polymers in order to prepare a master-batch to be added to granulate for compounding.
- In order to make them compatible with polymer of interest for MOMO, eventually new suitable coating for nanoparticles will be developed

Since the nanoparticles based composites are still in a primitive phase of study, a further scientific objective will be the development of test method suitable for them, in order to understand their real potential. We will analyse in depth:

- 1) Dispersion: to verify soft agglomeration is avoided
- 2) Functional and process properties: to verify their field of applications

Finally, project will be concretized in 3 technological objectives that are the set-up and optimisation of three different technologies:

- fibre spinning (it represents the most innovative technologies in nanocomposite field);
- injection moulding (for high volume production of car part);
- extrusion (profiles production).

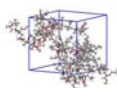
At the end of the project at least four demonstrators will be available to quantify the results.

Work performed

During the three years of the project all the goals identified in the technical annex has been perceived.

The goals are briefly summarised in the following list:

- **WP 1** – initial specification vs application and technologies
- **WP 2** – development of molecular modelling
- **WP 3** – compounding of recycled blends and nanocomposites
- **WP 4** – comparison between recycled and virgin properties of polymers characterisation of recycled materials developed
- **WP 5** – optimisation of technologies (fiber spinning, injection moulding, extrusion)



- **WP 6** – production of demonstrators
- **WP 7** – project management

Results achieved at the end of the project

The results achieved at the end of the project are reported in the following list:

- Fundamental knowledge concerning recycling of polymeric materials
- Development of modelling protocols for:
 - Pure polymers
 - Nanoclays
 - Compatibilization of clays
 - Polymeric blends
 - Polymeric nanocomposites
- Dedicated mesoscale code
- Fundamental knowledge concerning dispersion of nanoclays into polymers and polymers blends, in particular masterbatch production
- Recipes for specific recycled polymeric blends and nanocomposites
- Fundamental knowledge concerning processing of recycled materials with injection moulding, fiber spinning extrusion and casting
- Guidelines how to process with the abovementioned technologies recycled blends and nanocomposites
- Identification and realisation of possible industrial products (demonstrators) for the exploitation of project results.

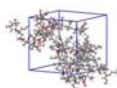
Expected end results

Expected end results of MOMO have been summarised in **Table 1**

Intentions for use and impact

Exploitation of MOMO results have been summarised in **Table 1**

EXPECTED RESULTS AND EXPLOITATION				
Project output/result	Range of applications	Expected impact	Timing	Main partners responsible for exploitation
Community added value				
“zero waste production”	Manufacturing industries	High	Medium Term	All partners
New field of application for nanoparticles	Nanotechnologies industries	High	Medium Term	All partners
Social/environmental (Community policies)				
New recycling techniques	Suppliers, processors, end users and consumers of nanocomposites	High	Medium Term	All partners
Technical				
Understanding phase behaviour and interfacial	Fundamental knowledge of nanocomposite	High	Medium Term	UNITS, WUT, UPV-EHU, NPI, CRP



phenomena				
Structure properties relationship	Fundamental knowledge of nanocomposite	High	Medium Term	All partners
Modelling procedures	Molecular modelling knowledge	High	Short Term	UNITS, UPV-EHU, CRP
Producing reclaimed nanocomposites (mastebatch, melt intercalation)	Nanotechnologies industries	High	Long Term	IFP SICOMP, CRP, WUT, NPI, POLY
Processing nanocomposites	Reliable production of high quality components for automotive and ophther manufacturing industries	Medium	Medium Term	IFP SICOMP, CRP, GP, M&P BURJA

Table 1 expected end results and exploitation

Project web site

A dedicated web space¹ has been created since third project month:

www.momoproject.org

WWW.MoMoProject.org

MOMO
INNOVATIVE MOLECULAR MODELLING APPROACH TO UP-GRADE POLYMERIC MATERIALS FROM POST INDUSTRIAL REJECTS

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Project will explore also how injection moulding, extrusion, and fibre spinning technologies

Fig. 1 Home page of MOMO web site

¹ A Dedicated Deliverable is available which elucidate how to navigate the web site :

<http://portal.momoproject.org/Deliverables/D%207%2015%20WEb%20page%20of%20the%20project.pdf>